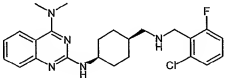
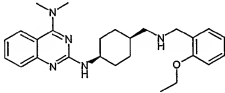
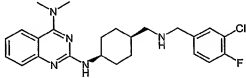
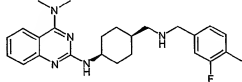
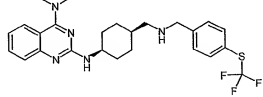
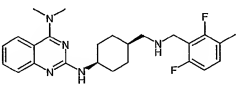
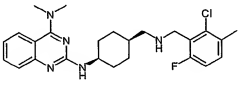
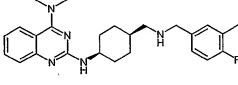
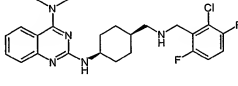
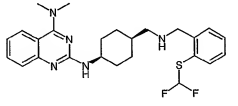
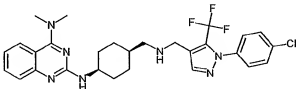
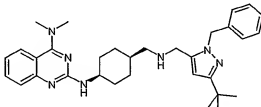
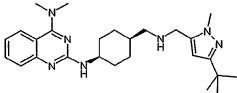
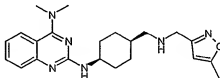
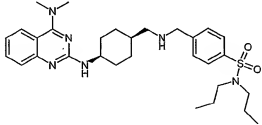


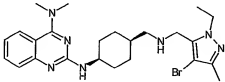
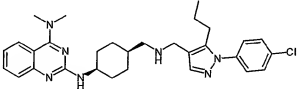
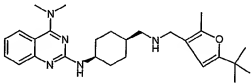
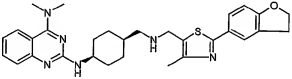
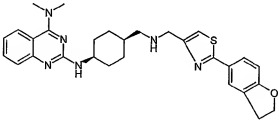
| Example No. | Structure  | APCI-MS     |
|-------------|--|-------------|
| 1297        |   | 442 (M + H) |
| 1298        |   | 434 (M + H) |
| 1299        |   | 442 (M + H) |
| 1300        |   | 422 (M + H) |
| 1301        |  | 490 (M + H) |

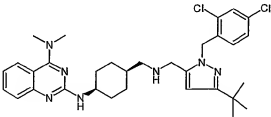
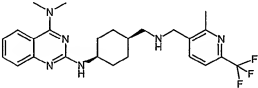
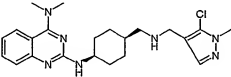
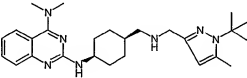
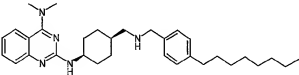
| Example No. | Structure  | APCI-MS     |
|-------------|--|-------------|
| 1302        |   | 440 (M + H) |
| 1303        |   | 456 (M + H) |
| 1304        |   | 422 (M + H) |
| 1305        |   | 460 (M + H) |
| 1306        |  | 472 (M + H) |

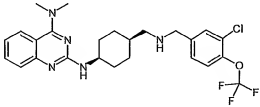
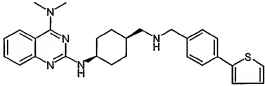
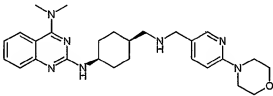
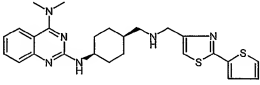
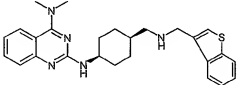
| Example No. | Structure  | APCI-MS     |
|-------------|--|-------------|
| 1307        | <br><chem>CN(C)c1nc2ccccc2n1NC3CCCCC3CNC4CC(C4)CNC5C(Cl)C(Cl)C(Cl)S5</chem>      | 498 (M + H) |
| 1308        | <br><chem>CN(C)c1nc2ccccc2n1NC3CCCCC3CNC4CC(C4)CNC5C(Cl)C(Cl)CSC5</chem>         | 464 (M + H) |
| 1309        | <br><chem>CN(C)c1nc2ccccc2n1NC3CCCCC3CNC4CC(C4)CNC5C(C)C(C)CSC5</chem>           | 418 (M + H) |
| 1310        | <br><chem>CN(C)c1nc2ccccc2n1NC3CCCCC3CNC4CC(C4)CNC5C(Cl)C(Cl)C5C6C(C)COC6</chem> | 539 (M + H) |
| 1311        | <br><chem>CN(C)c1nc2ccccc2n1NC3CCCCC3CNC4CC(C4)CNC5C(OC6=CC=C(C=C6))C5</chem>    | 497 (M + H) |

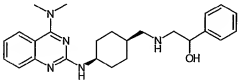
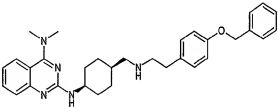
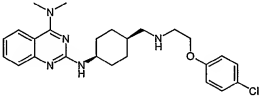
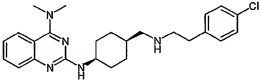
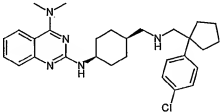
| Example No. | Structure  | APCI-MS     |
|-------------|--|-------------|
| 1312        |   | 558 (M + H) |
| 1313        |   | 526 (M + H) |
| 1314        |   | 450 (M + H) |
| 1315        |   | 395 (M + H) |
| 1316        |  | 553 (M + H) |

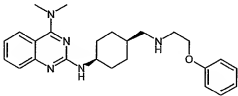
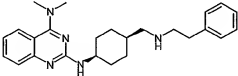
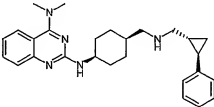
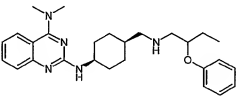
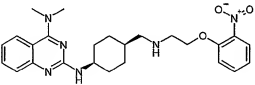


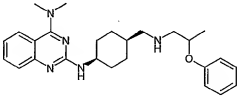
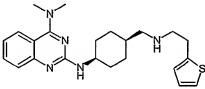
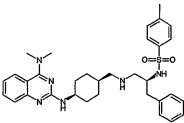
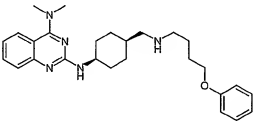
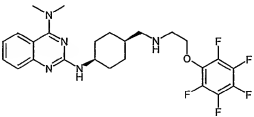
| Example No. | Structure  | APCI-MS     |
|-------------|--|-------------|
| 1317        |   | 500 (M + H) |
| 1318        |   | 532 (M + H) |
| 1319        |   | 450 (M + H) |
| 1320        |   | 529 (M + H) |
| 1321        |  | 515 (M + H) |

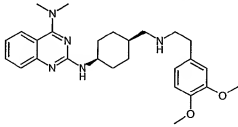
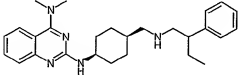
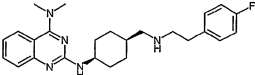
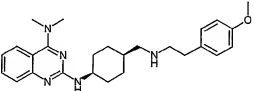
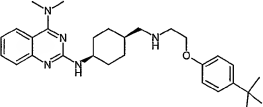
| Example No. | Structure  | APCI-MS     |
|-------------|--|-------------|
| 1322        |   | 594 (M + H) |
| 1323        |   | 473 (M + H) |
| 1324        |   | 428 (M + H) |
| 1325        |   | 450 (M + H) |
| 1326        |  | 502 (M + H) |

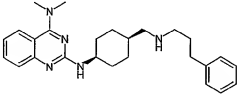
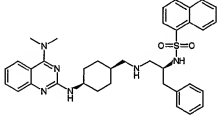
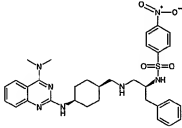
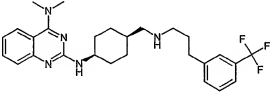
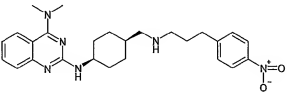
| Example No. | Structure  | APCI-MS     |
|-------------|--|-------------|
| 1327        |   | 508 (M + H) |
| 1328        |   | 472 (M + H) |
| 1329        |   | 476 (M + H) |
| 1330        |   | 479 (M + H) |
| 1331        |  | 446 (M + H) |

| Example No. | Structure  | APCI-MS     |
|-------------|--|-------------|
| 1332        |   | 420 (M + H) |
| 1333        |   | 510 (M + H) |
| 1334        |   | 454 (M + H) |
| 1335        |   | 438 (M + H) |
| 1336        |  | 492 (M + H) |

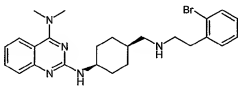
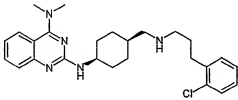
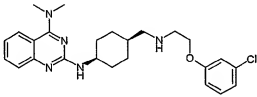
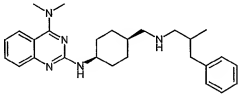
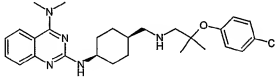
| Example No. | Structure  | APCI-MS     |
|-------------|--|-------------|
| 1337        |   | 420 (M + H) |
| 1338        |   | 404 (M + H) |
| 1339        |   | 430 (M + H) |
| 1340        |   | 448 (M + H) |
| 1341        |  | 465 (M + H) |

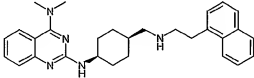
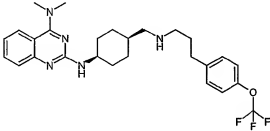
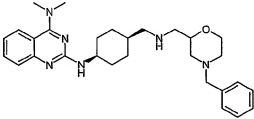
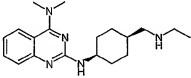
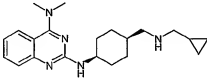
| Example No. | Structure  | APCI-MS     |
|-------------|--|-------------|
| 1342        |   | 434 (M + H) |
| 1343        |   | 410 (M + H) |
| 1344        |   | 587 (M + H) |
| 1345        |   | 448 (M + H) |
| 1346        |  | 510 (M + H) |

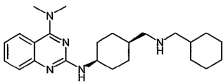
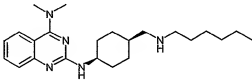
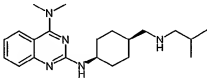
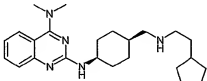
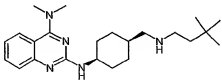
| Example No. | Structure  | APCI-MS     |
|-------------|--|-------------|
| 1347        |   | 464 (M + H) |
| 1348        |   | 432 (M + H) |
| 1349        |   | 422 (M + H) |
| 1350        |   | 434 (M + H) |
| 1351        |  | 476 (M + H) |

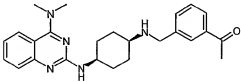
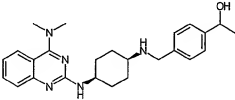
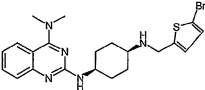
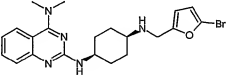
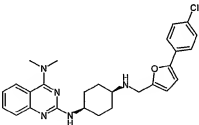
| Example No. | Structure  | APCI-MS   |
|-------------|--|-----------|
| 1352        |   | 418 (M+H) |
| 1353        |   | 623 (M+H) |
| 1354        |   | 618 (M+H) |
| 1355        |   | 486 (M+H) |
| 1356        |  | 463 (M+H) |

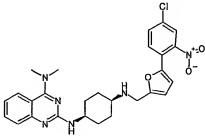
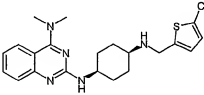
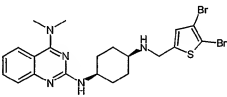
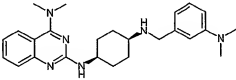
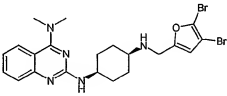


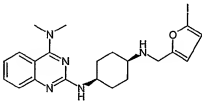
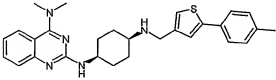
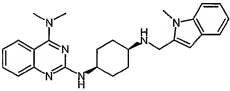
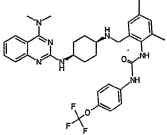
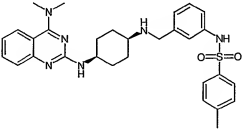
| Example No. | Structure  | APCI-MS     |
|-------------|--|-------------|
| 1357        |   | 482 (M + H) |
| 1358        |   | 452 (M + H) |
| 1359        |   | 454 (M + H) |
| 1360        |   | 432 (M + H) |
| 1361        |  | 482 (M + H) |

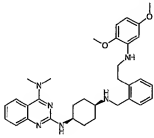
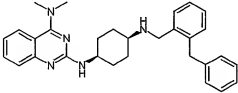
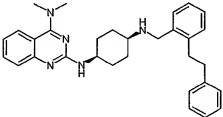
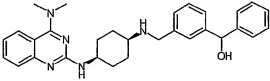
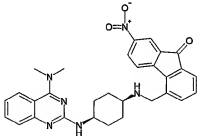
| Example No. | Structure  | APCI-MS     |
|-------------|--|-------------|
| 1362        |   | 454 (M + H) |
| 1363        |   | 502 (M + H) |
| 1364        |   | 489 (M + H) |
| 1365        |   | 328 (M + H) |
| 1366        |  | 354 (M + H) |

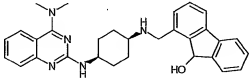
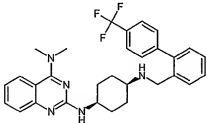
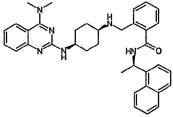
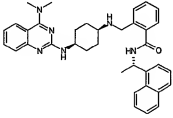
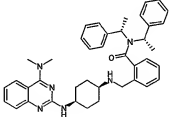
| Example No. | Structure  | APCI-MS     |
|-------------|--|-------------|
| 1367        |   | 396 (M + H) |
| 1368        |   | 384 (M + H) |
| 1369        |   | 356 (M + H) |
| 1370        |   | 396 (M + H) |
| 1371        |  | 384 (M + H) |

| Example No. | Structure  | APCI-MS     |
|-------------|--|-------------|
| 1372        |   | 418 (M + H) |
| 1373        |   | 420 (M + H) |
| 1374        |   | 460 (M + H) |
| 1375        |   | 444 (M + H) |
| 1376        |  | 476 (M + H) |

| Example No. | Structure  | APCI-MS     |
|-------------|--|-------------|
| 1377        |   | 521 (M + H) |
| 1378        |   | 416 (M + H) |
| 1379        |   | 538 (M + H) |
| 1380        |   | 419 (M + H) |
| 1381        |  | 522 (M + H) |

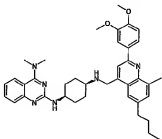
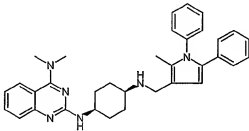
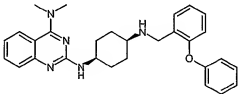
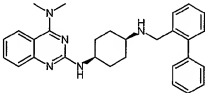
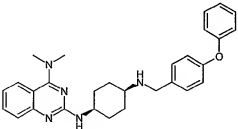
| Example No. | Structure  | APCI-MS     |
|-------------|--|-------------|
| 1382        |   | 492 (M + H) |
| 1383        |   | 472 (M + H) |
| 1384        |   | 429 (M + H) |
| 1385        |   | 622 (M + H) |
| 1386        |  | 545 (M + H) |

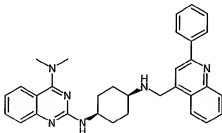
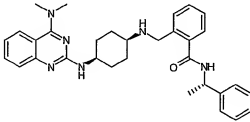
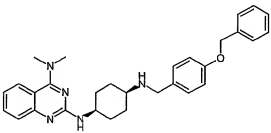
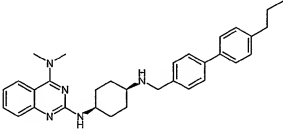
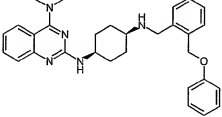
| Example No. | Structure  | APCI-MS     |
|-------------|--|-------------|
| 1387        |   | 555 (M + H) |
| 1388        |   | 466 (M + H) |
| 1389        |   | 480 (M + H) |
| 1390        |   | 482 (M + H) |
| 1391        |  | 523 (M + H) |

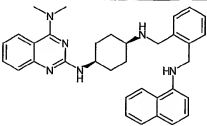
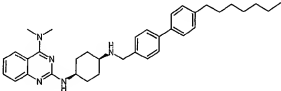
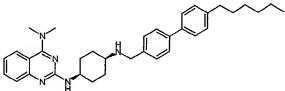
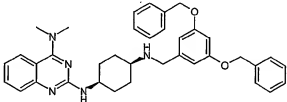
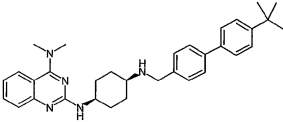
| Example No. | Structure  | APCI-MS     |
|-------------|--|-------------|
| 1392        |   | 480 (M + H) |
| 1393        |   | 520 (M + H) |
| 1394        |   | 573 (M + H) |
| 1395        |   | 573 (M + H) |
| 1396        |  | 627 (M + H) |

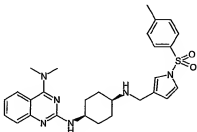
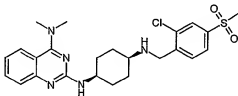
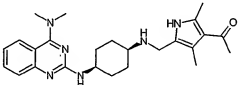
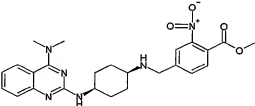
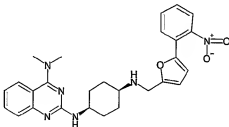


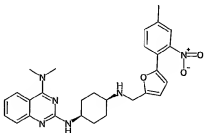
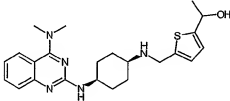
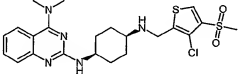
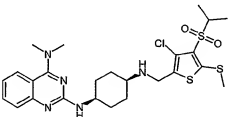
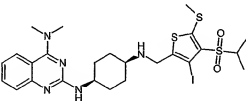


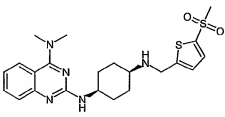
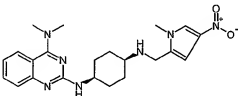
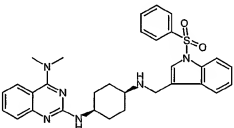
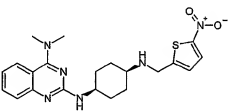
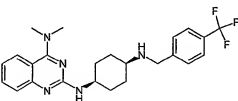
| Example No. | Structure  | APCI-MS     |
|-------------|--|-------------|
| 1402        |   | 633 (M + H) |
| 1403        |   | 531 (M + H) |
| 1404        |   | 468 (M + H) |
| 1405        |   | 452 (M + H) |
| 1406        |  | 468 (M + H) |

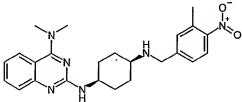
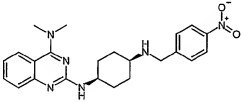
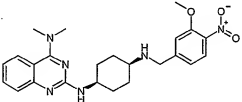
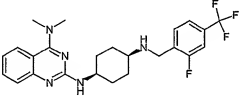
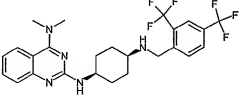
| Example No. | Structure  | APCI-MS     |
|-------------|--|-------------|
| 1407        |   | 503 (M + H) |
| 1408        |   | 523 (M + H) |
| 1409        |   | 482 (M + H) |
| 1410        |   | 494 (M + H) |
| 1411        |  | 482 (M + H) |

| Example No. | Structure  | APCI-MS     |
|-------------|--|-------------|
| 1412        |   | 531 (M + H) |
| 1413        |   | 550 (M + H) |
| 1414        |   | 536 (M + H) |
| 1415        |   | 588 (M + H) |
| 1416        |  | 508 (M + H) |

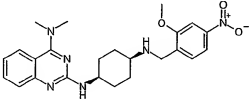
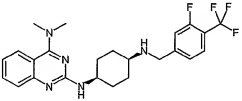
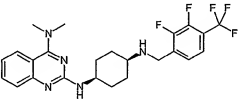
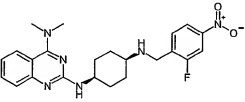
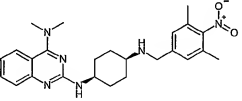
| Example No. | Structure  | APCI-MS     |
|-------------|--|-------------|
| 1417        |   | 519 (M + H) |
| 1418        |   | 488 (M + H) |
| 1419        |   | 435 (M + H) |
| 1420        |   | 479 (M + H) |
| 1421        |  | 487 (M + H) |

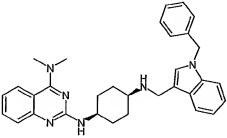
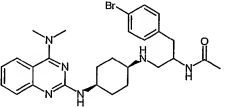
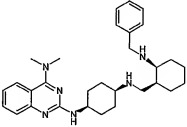
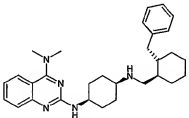
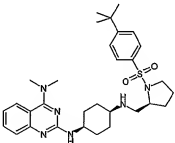
| Example No. | Structure  | APCI-MS     |
|-------------|--|-------------|
| 1422        |   | 501 (M + H) |
| 1423        |   | 426 (M + H) |
| 1424        |   | 494 (M + H) |
| 1425        |   | 568 (M + H) |
| 1426        |  | 660 (M + H) |

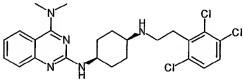
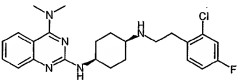
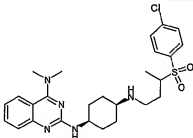
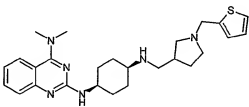
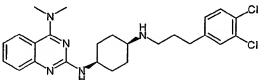
| Example No. | Structure  | APCI-MS     |
|-------------|--|-------------|
| 1427        |   | 460 (M + H) |
| 1428        |   | 424 (M + H) |
| 1429        |   | 555 (M + H) |
| 1430        |   | 427 (M + H) |
| 1431        |  | 444 (M + H) |

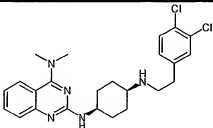
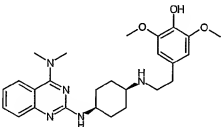
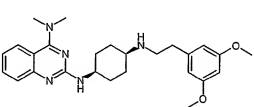
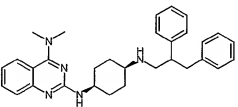
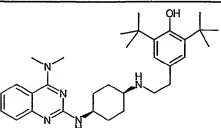
| Example No. | Structure  | APCI-MS     |
|-------------|--|-------------|
| 1432        |   | 435 (M + H) |
| 1433        |   | 421 (M + H) |
| 1434        |   | 451 (M + H) |
| 1435        |   | 462 (M + H) |
| 1436        |  | 512 (M + H) |

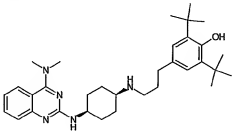
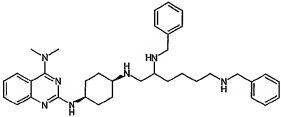
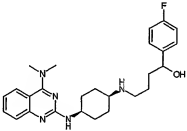
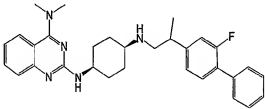
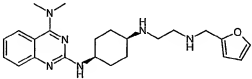


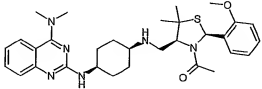
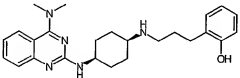
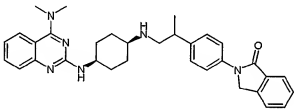
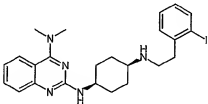
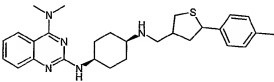
| Example No. | Structure  | APCI-MS     |
|-------------|--|-------------|
| 1437        |   | 451 (M + H) |
| 1438        |   | 462 (M + H) |
| 1439        |   | 480 (M + H) |
| 1440        |   | 439 (M + H) |
| 1441        |  | 449 (M + H) |

| Example No. | Structure  | APCI-MS     |
|-------------|--|-------------|
| 1442        |   | 505 (M + H) |
| 1443        |   | 539 (M + H) |
| 1444        |   | 487 (M + H) |
| 1445        |   | 488 (M + H) |
| 1446        |  | 565 (M + H) |

| Example No. | Structure  | APCI-MS     |
|-------------|--|-------------|
| 1447        |   | 492 (M + H) |
| 1448        |   | 442 (M + H) |
| 1449        |   | 516 (M + H) |
| 1450        |   | 465 (M + H) |
| 1451        |  | 472 (M + H) |

| Example No. | Structure  | APCI-MS     |
|-------------|--|-------------|
| 1452        |   | 458 (M + H) |
| 1453        |   | 466 (M + H) |
| 1454        |   | 450 (M + H) |
| 1455        |   | 480 (M + H) |
| 1456        |  | 518 (M + H) |

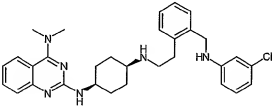
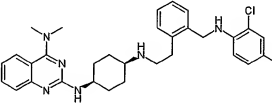
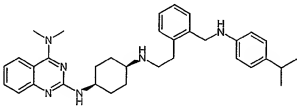
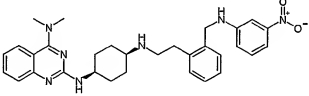
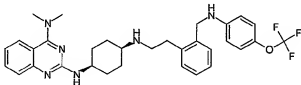
| Example No. | Structure  | APCI-MS     |
|-------------|--|-------------|
| 1457        |   | 532 (M + H) |
| 1458        |   | 580 (M + H) |
| 1459        |   | 452 (M + H) |
| 1460        |   | 498 (M + H) |
| 1461        |  | 409 (M + H) |

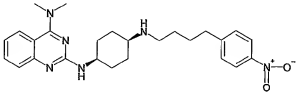
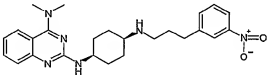
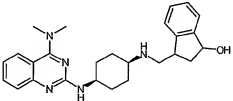
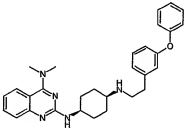
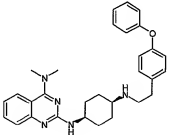
| Example No. | Structure  | APCI-MS     |
|-------------|--|-------------|
| 1462        |   | 563 (M + H) |
| 1463        |   | 420 (M + H) |
| 1464        |   | 535 (M + H) |
| 1465        |   | 516 (M + H) |
| 1466        |  | 476 (M + H) |

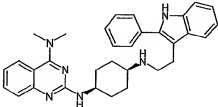
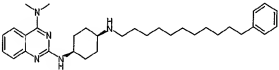
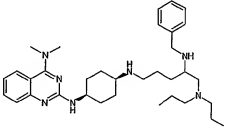
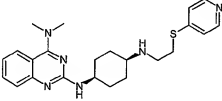
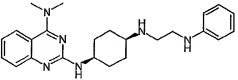


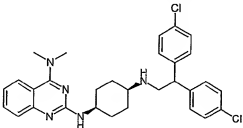
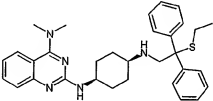
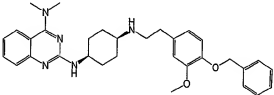
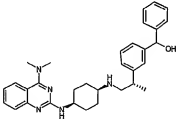
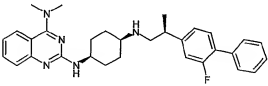
| Example No. | Structure | APCI-MS     |
|-------------|-----------|-------------|
| 1472        |           | 648 (M + H) |
| 1473        |           | 591 (M + H) |
| 1474        |           | 645 (M + H) |
| 1475        |           | 531 (M + H) |
| 1476        |           | 619 (M + H) |

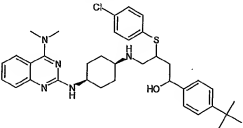
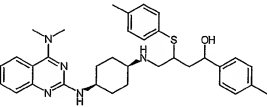
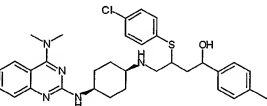
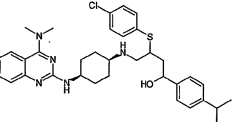
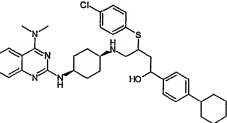


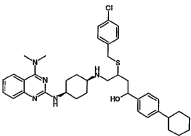
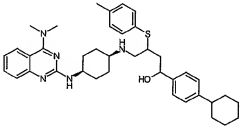
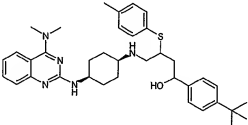
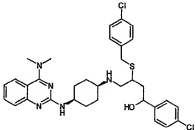
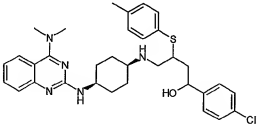
| Example No. | Structure  | APCI-MS     |
|-------------|--|-------------|
| 1477        |   | 529 (M + H) |
| 1478        |   | 563 (M + H) |
| 1479        |   | 537 (M + H) |
| 1480        |   | 540 (M + H) |
| 1481        |  | 579 (M + H) |

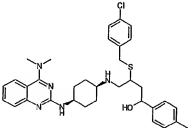
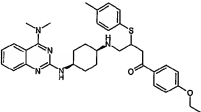
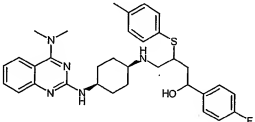
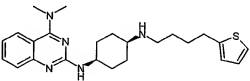
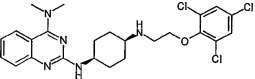
| Example No. | Structure  | APCI-MS     |
|-------------|--|-------------|
| 1482        |   | 463 (M + H) |
| 1483        |   | 449 (M + H) |
| 1484        |   | 432 (M + H) |
| 1485        |   | 482 (M + H) |
| 1486        |  | 482 (M + H) |

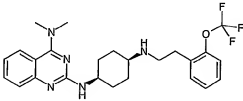
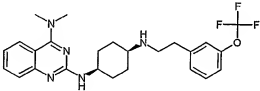
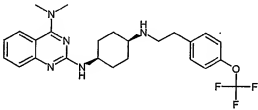
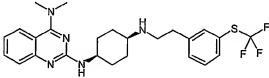
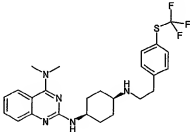
| Example No. | Structure  | APCI-MS     |
|-------------|--|-------------|
| 1487        |   | 505 (M + H) |
| 1488        |   | 516 (M + H) |
| 1489        |   | 560 (M + H) |
| 1490        |   | 423 (M + H) |
| 1491        |  | 405 (M + H) |

| Example No. | Structure  | APCI-MS     |
|-------------|--|-------------|
| 1492        |   | 534 (M + H) |
| 1493        |   | 526 (M + H) |
| 1494        |   | 526 (M + H) |
| 1495        |   | 510 (M + H) |
| 1496        |  | 498 (M + H) |

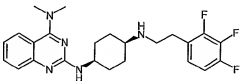
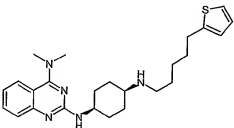
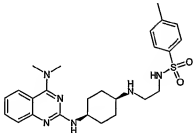
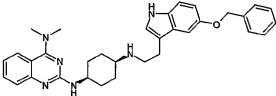
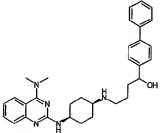
| Example No. | Structure  | APCI-MS     |
|-------------|--|-------------|
| 1497        |   | 632 (M + H) |
| 1498        |   | 570 (M + H) |
| 1499        |   | 590 (M + H) |
| 1500        |   | 618 (M + H) |
| 1501        |  | 658 (M + H) |

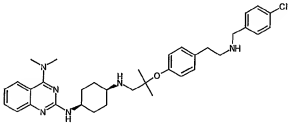
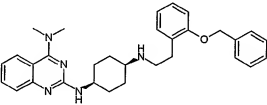
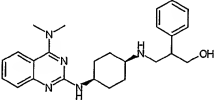
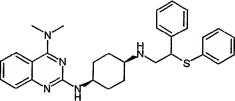
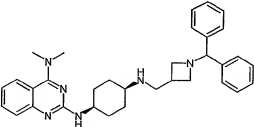
| Example No. | Structure  | APCI-MS     |
|-------------|--|-------------|
| 1502        |   | 672 (M + H) |
| 1503        |   | 638 (M + H) |
| 1504        |   | 612 (M + H) |
| 1505        |   | 624 (M + H) |
| 1506        |  | 590 (M + H) |

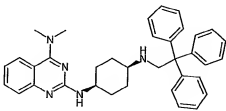
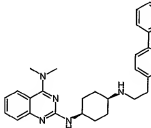
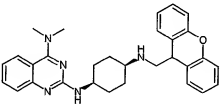
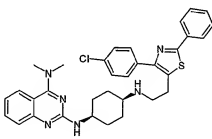
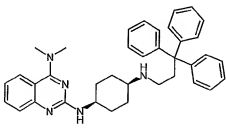
| Example No. | Structure  | APCI-MS     |
|-------------|--|-------------|
| 1507        |   | 604 (M + H) |
| 1508        |   | 598 (M + H) |
| 1509        |   | 574 (M + H) |
| 1510        |   | 424 (M + H) |
| 1511        |  | 508 (M + H) |

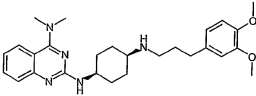
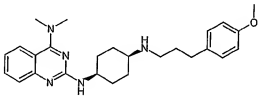
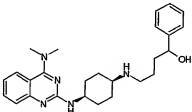
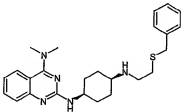
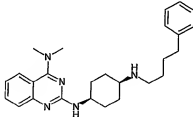
| Example No. | Structure  | APCI-MS     |
|-------------|--|-------------|
| 1512        |   | 474 (M + H) |
| 1513        |   | 474 (M + H) |
| 1514        |   | 474 (M + H) |
| 1515        |   | 490 (M + H) |
| 1516        |  | 490 (M + H) |

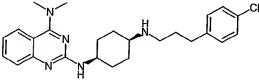
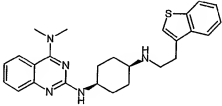
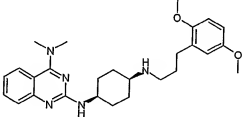
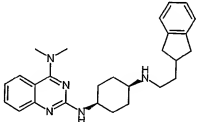
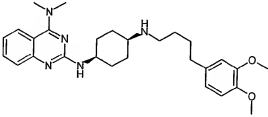


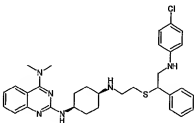
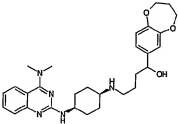
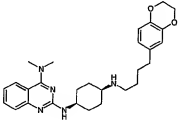
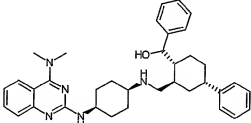
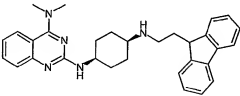
| Example No. | Structure  | APCI-MS     |
|-------------|--|-------------|
| 1517        |   | 444 (M + H) |
| 1518        |   | 438 (M + H) |
| 1519        |   | 483 (M + H) |
| 1520        |   | 535 (M + H) |
| 1521        |  | 510 (M + H) |

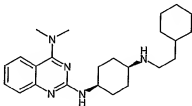
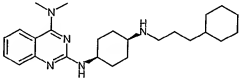
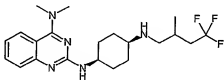
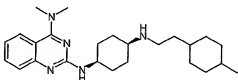
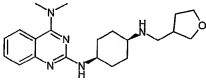
| Example No. | Structure  | APCI-MS     |
|-------------|--|-------------|
| 1522        |   | 601 (M + H) |
| 1523        |   | 496 (M + H) |
| 1524        |   | 420 (M + H) |
| 1525        |   | 498 (M + H) |
| 1526        |  | 521 (M + H) |

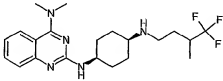
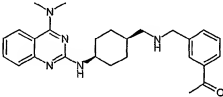
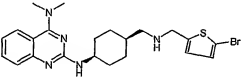
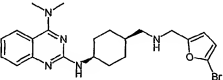
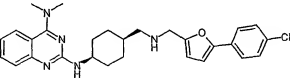
| Example No. | Structure  | APCI-MS     |
|-------------|--|-------------|
| 1527        |   | 542 (M + H) |
| 1528        |   | 466 (M + H) |
| 1529        |   | 480 (M + H) |
| 1530        |   | 583 (M + H) |
| 1531        |  | 556 (M + H) |

| Example No. | Structure  | APCI-MS     |
|-------------|--|-------------|
| 1532        |   | 464 (M + H) |
| 1533        |   | 434 (M + H) |
| 1534        |   | 434 (M + H) |
| 1535        |   | 436 (M + H) |
| 1536        |  | 418 (M + H) |

| Example No. | Structure  | APCI-MS     |
|-------------|--|-------------|
| 1537        |   | 438 (M + H) |
| 1538        |   | 446 (M + H) |
| 1539        |   | 464 (M + H) |
| 1540        |   | 430 (M + H) |
| 1541        |  | 478 (M + H) |

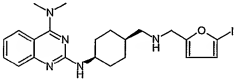
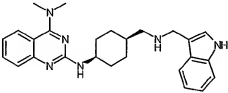
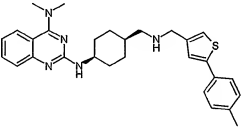
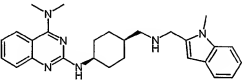
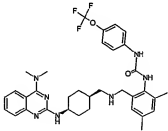
| Example No. | Structure  | APCI-MS     |
|-------------|--|-------------|
| 1542        |   | 575 (M + H) |
| 1543        |   | 506 (M + H) |
| 1544        |   | 476 (M + H) |
| 1545        |   | 564 (M + H) |
| 1546        |  | 478 (M + H) |

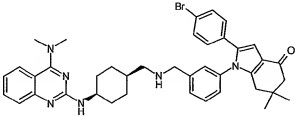
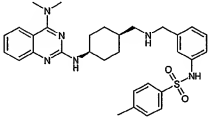
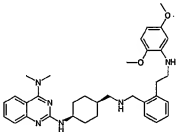
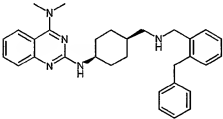
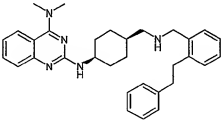
| Example No. | Structure  | APCI-MS     |
|-------------|--|-------------|
| 1547        |   | 396 (M + H) |
| 1548        |   | 410 (M + H) |
| 1549        |   | 410 (M + H) |
| 1550        |   | 410 (M + H) |
| 1551        |  | 370 (M + H) |

| Example No. | Structure  | APCI-MS     |
|-------------|--|-------------|
| 1552        |   | 410 (M + H) |
| 1553        |   | 432 (M + H) |
| 1554        |   | 474 (M + H) |
| 1555        |   | 458 (M + H) |
| 1556        |  | 490 (M + H) |

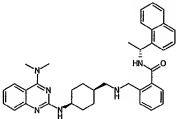
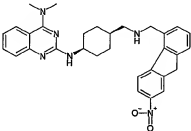
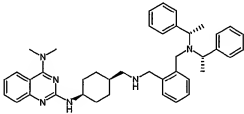
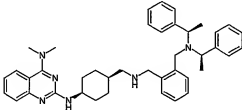
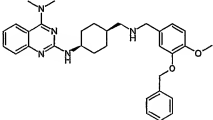




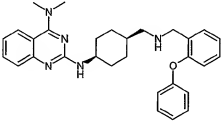
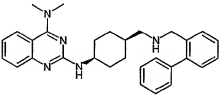
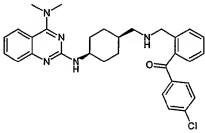
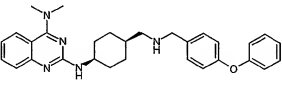
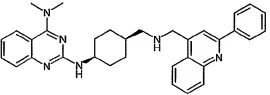
| Example No. | Structure  | APCI-MS     |
|-------------|--|-------------|
| 1562        |   | 506 (M + H) |
| 1563        |   | 429 (M + H) |
| 1564        |   | 486 (M + H) |
| 1565        |   | 443 (M + H) |
| 1566        |  | 636 (M + H) |

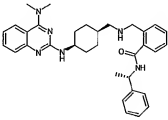
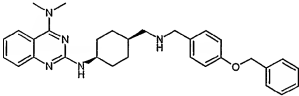
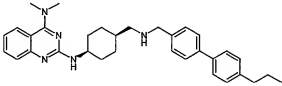
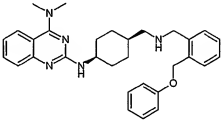
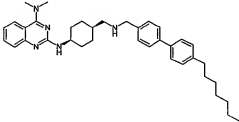
| Example No. | Structure  | APCI-MS     |
|-------------|--|-------------|
| 1567        |   | 705 (M + H) |
| 1568        |   | 559 (M + H) |
| 1569        |   | 569 (M + H) |
| 1570        |   | 480 (M + H) |
| 1571        |  | 494 (M + H) |



| Example No. | Structure  | APCI-MS     |
|-------------|--|-------------|
| 1577        |   | 587 (M + H) |
| 1578        |   | 523 (M + H) |
| 1579        |   | 627 (M + H) |
| 1580        |   | 627 (M + H) |
| 1581        |  | 526 (M + H) |

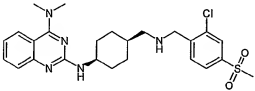
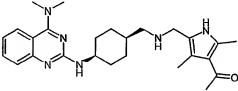
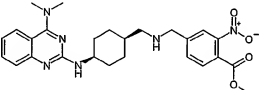
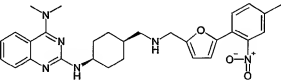
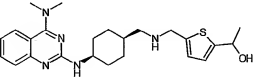


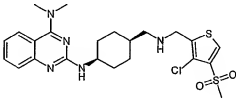
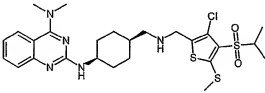
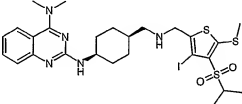
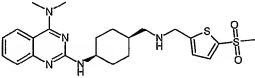
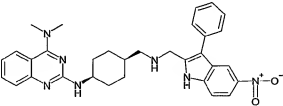
| Example No. | Structure  | APCI-MS     |
|-------------|--|-------------|
| 1587        |   | 482 (M + H) |
| 1588        |   | 466 (M + H) |
| 1589        |   | 528 (M + H) |
| 1590        |   | 482 (M + H) |
| 1591        |  | 517 (M + H) |

| Example No. | Structure  | APCI-MS     |
|-------------|--|-------------|
| 1592        |   | 537 (M + H) |
| 1593        |   | 496 (M + H) |
| 1594        |   | 508 (M + H) |
| 1595        |   | 496 (M + H) |
| 1596        |  | 564 (M + H) |

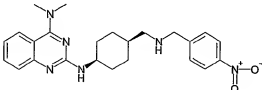
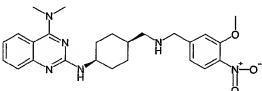
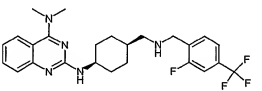
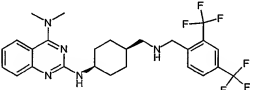
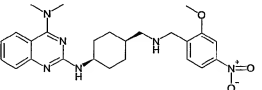


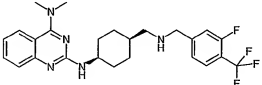
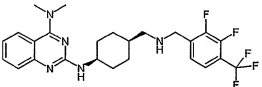
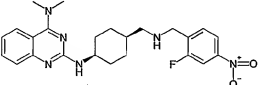
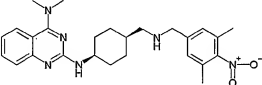
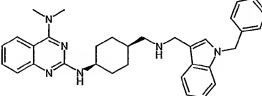


| Example No. | Structure  | APCI-MS     |
|-------------|--|-------------|
| 1602        |   | 502 (M + H) |
| 1603        |   | 449 (M + H) |
| 1604        |   | 493 (M + H) |
| 1605        |   | 515 (M + H) |
| 1606        |  | 440 (M + H) |

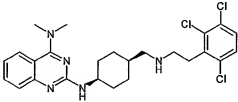
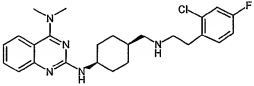
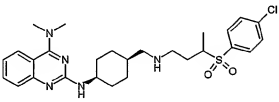
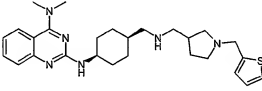
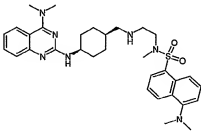
| Example No. | Structure  | APCI-MS     |
|-------------|--|-------------|
| 1607        |   | 508 (M + H) |
| 1608        |   | 582 (M + H) |
| 1609        |   | 674 (M + H) |
| 1610        |   | 474 (M + H) |
| 1611        |  | 548 (M - H) |



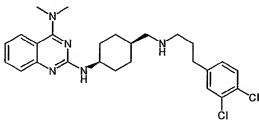
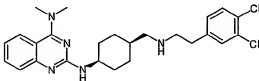
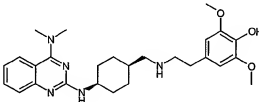
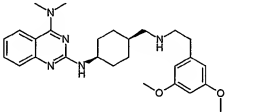
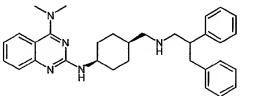
| Example No. | Structure  | APCI-MS     |
|-------------|--|-------------|
| 1617        |   | 435 (M + H) |
| 1618        |   | 465 (M + H) |
| 1619        |   | 476 (M + H) |
| 1620        |   | 526 (M + H) |
| 1621        |  | 465 (M + H) |

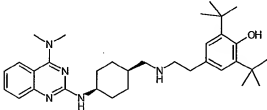
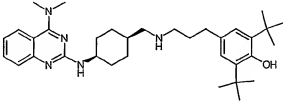
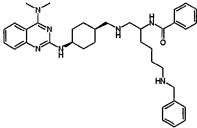
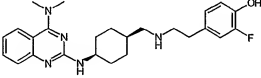
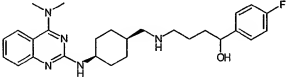
| Example No. | Structure  | APCI-MS     |
|-------------|--|-------------|
| 1622        |   | 476 (M + H) |
| 1623        |   | 494 (M + H) |
| 1624        |   | 453 (M + H) |
| 1625        |   | 463 (M + H) |
| 1626        |  | 519 (M + H) |

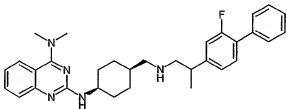
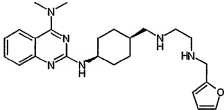
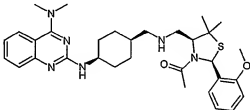
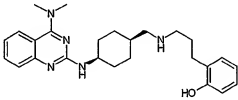
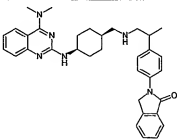


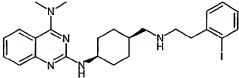
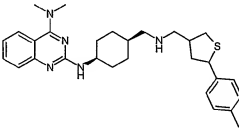
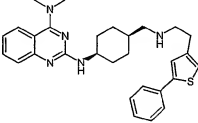
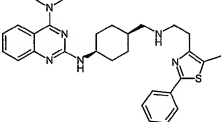
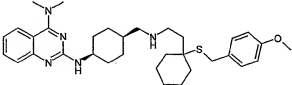
| Example No. | Structure  | APCI-MS     |
|-------------|--|-------------|
| 1632        |   | 506 (M + H) |
| 1633        |   | 456 (M + H) |
| 1634        |   | 530 (M + H) |
| 1635        |   | 479 (M + H) |
| 1636        |  | 590 (M + H) |

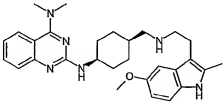
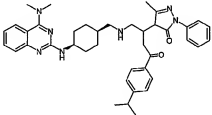
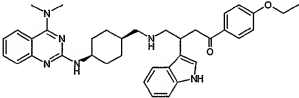
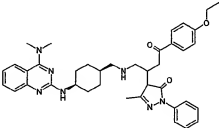
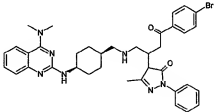


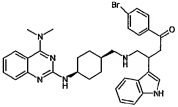
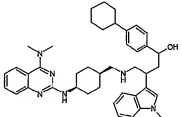
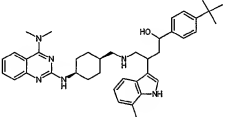
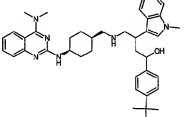
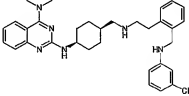
| Example No. | Structure  | APCI-MS     |
|-------------|--|-------------|
| 1637        |   | 486 (M + H) |
| 1638        |   | 472 (M + H) |
| 1639        |   | 480 (M + H) |
| 1640        |   | 464 (M + H) |
| 1641        |  | 494 (M + H) |

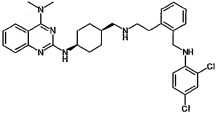
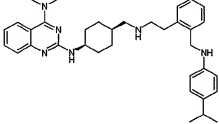
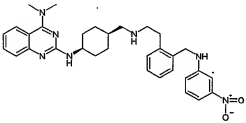
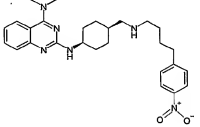
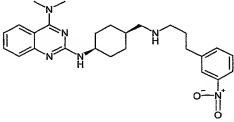
| Example No. | Structure  | APCI-MS     |
|-------------|--|-------------|
| 1642        |   | 532 (M + H) |
| 1643        |   | 546 (M + H) |
| 1644        |   | 608 (M + H) |
| 1645        |   | 438 (M + H) |
| 1646        |  | 466 (M + H) |

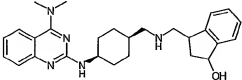
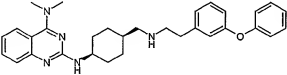
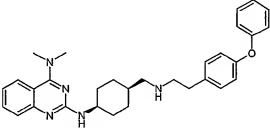
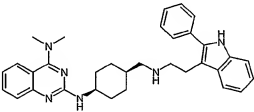
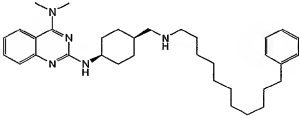
| Example No. | Structure  | APCI-MS     |
|-------------|--|-------------|
| 1647        |   | 512 (M + H) |
| 1648        |   | 423 (M + H) |
| 1649        |   | 577 (M + H) |
| 1650        |   | 434 (M + H) |
| 1651        |  | 549 (M + H) |

| Example No. | Structure  | APCI-MS     |
|-------------|--|-------------|
| 1652        |   | 530 (M + H) |
| 1653        |   | 490 (M + H) |
| 1654        |   | 486 (M + H) |
| 1655        |   | 501 (M + H) |
| 1656        |  | 562 (M + H) |

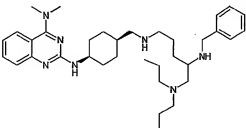
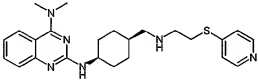
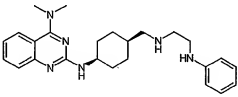
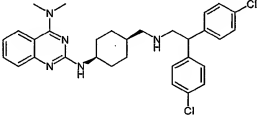
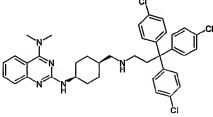
| Example No. | Structure  | APCI-MS     |
|-------------|--|-------------|
| 1657        |   | 487 (M + H) |
| 1658        |   | 660 (M + H) |
| 1659        |   | 605 (M + H) |
| 1660        |   | 662 (M + H) |
| 1661        |  | 696 (M + H) |

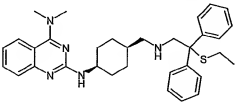
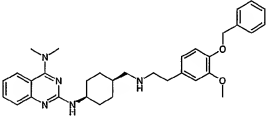
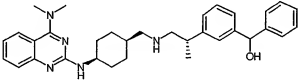
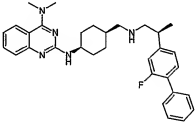
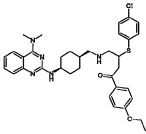
| Example No. | Structure  | APCI-MS     |
|-------------|--|-------------|
| 1662        |   | 639 (M + H) |
| 1663        |   | 659 (M + H) |
| 1664        |   | 647 (M + H) |
| 1665        |   | 633 (M + H) |
| 1666        |  | 543 (M + H) |

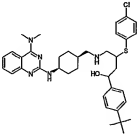
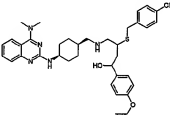
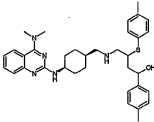
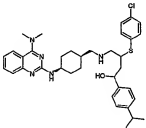
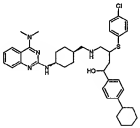
| Example No. | Structure  | APCI-MS     |
|-------------|--|-------------|
| 1667        |   | 577 (M + H) |
| 1668        |   | 551 (M + H) |
| 1669        |   | 554 (M + H) |
| 1670        |   | 477 (M + H) |
| 1671        |  | 463 (M + H) |

| Example No. | Structure  | APCI-MS     |
|-------------|--|-------------|
| 1672        |   | 446 (M + H) |
| 1673        |   | 496 (M + H) |
| 1674        |   | 496 (M + H) |
| 1675        |   | 519 (M + H) |
| 1676        |  | 530 (M + H) |

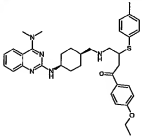
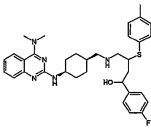
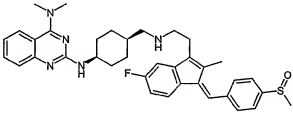
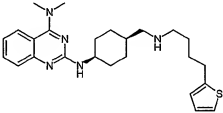
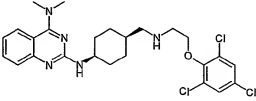


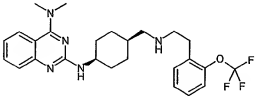
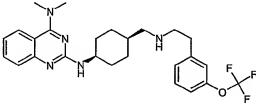
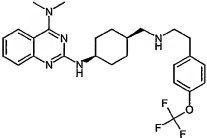
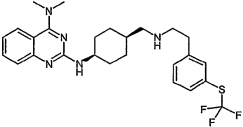
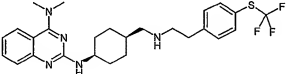
| Example No. | Structure  | APCI-MS     |
|-------------|--|-------------|
| 1677        |   | 574 (M + H) |
| 1678        |   | 437 (M + H) |
| 1679        |   | 419 (M + H) |
| 1680        |   | 548 (M + H) |
| 1681        |  | 672 (M + H) |

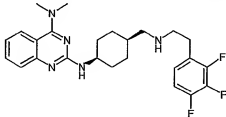
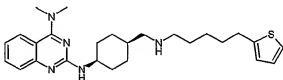
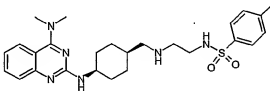
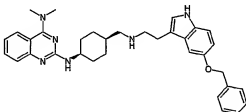
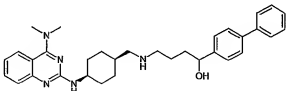
| Example No. | Structure  | APCI-MS     |
|-------------|--|-------------|
| 1682        |   | 540 (M + H) |
| 1683        |   | 540 (M + H) |
| 1684        |   | 524 (M + H) |
| 1685        |   | 512 (M + H) |
| 1686        |  | 632 (M + H) |

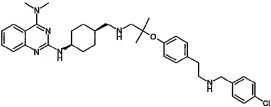
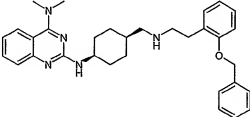
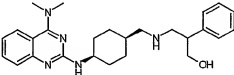
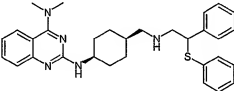
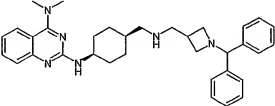
| Example No. | Structure  | APCI-MS     |
|-------------|--|-------------|
| 1687        |   | 646 (M + H) |
| 1688        |   | 648 (M + H) |
| 1689        |   | 584 (M + H) |
| 1690        |   | 632 (M + H) |
| 1691        |  | 672 (M + H) |



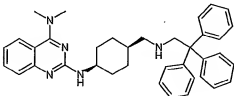
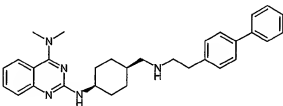
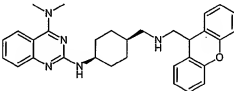
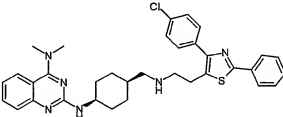
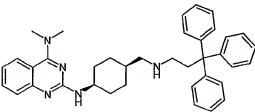
| Example No. | Structure  | APCI-MS     |
|-------------|--|-------------|
| 1697        |   | 612 (M + H) |
| 1698        |   | 588 (M + H) |
| 1699        |   | 624 (M + H) |
| 1700        |   | 438 (M + H) |
| 1701        |  | 522 (M + H) |

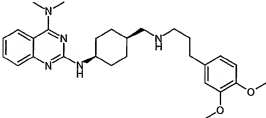
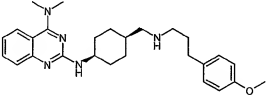
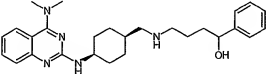
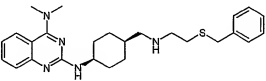
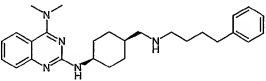
| Example No. | Structure  | APCI-MS     |
|-------------|--|-------------|
| 1702        |   | 488 (M + H) |
| 1703        |   | 488 (M + H) |
| 1704        |   | 488 (M + H) |
| 1705        |   | 504 (M + H) |
| 1706        |  | 504 (M + H) |

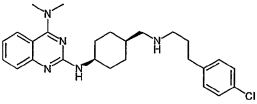
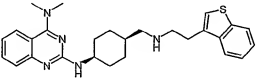
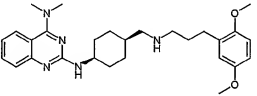
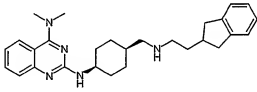
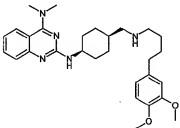
| Example No. | Structure  | APCI-MS     |
|-------------|--|-------------|
| 1707        |   | 458 (M + H) |
| 1708        |   | 452 (M + H) |
| 1709        |   | 497 (M + H) |
| 1710        |   | 549 (M + H) |
| 1711        |  | 524 (M + H) |

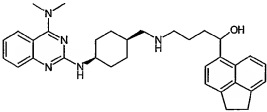
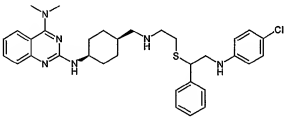
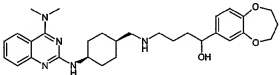
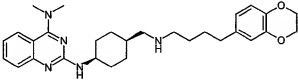
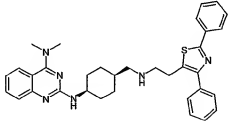
| Example No. | Structure  | APCI-MS     |
|-------------|--|-------------|
| 1712        |   | 615 (M + H) |
| 1713        |   | 510 (M + H) |
| 1714        |   | 434 (M + H) |
| 1715        |   | 512 (M + H) |
| 1716        |  | 535 (M + H) |

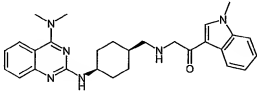
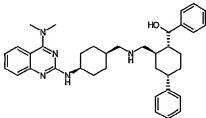
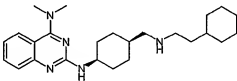
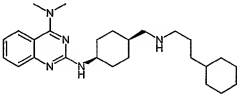
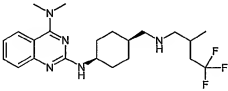


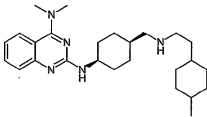
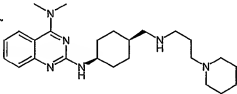
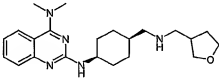
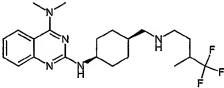
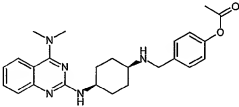
| Example No. | Structure  | APCI-MS     |
|-------------|--|-------------|
| 1717        |   | 556 (M + H) |
| 1718        |   | 480 (M + H) |
| 1719        |   | 494 (M + H) |
| 1720        |   | 597 (M + H) |
| 1721        |  | 570 (M + H) |

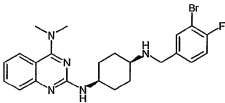
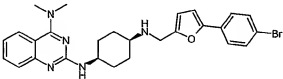
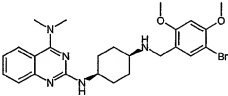
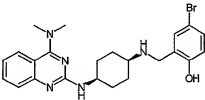
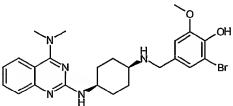
| Example No. | Structure  | APCI-MS     |
|-------------|--|-------------|
| 1722        |   | 478 (M + H) |
| 1723        |   | 448 (M + H) |
| 1724        |   | 448 (M + H) |
| 1725        |   | 450 (M + H) |
| 1726        |  | 432 (M + H) |

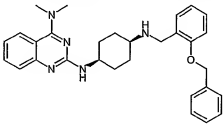
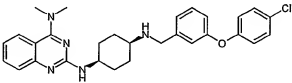
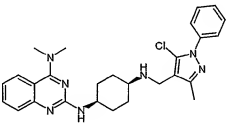
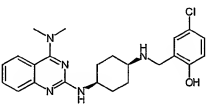
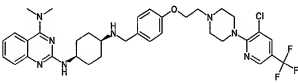
| Example No. | Structure  | APCI-MS     |
|-------------|--|-------------|
| 1727        |   | 452 (M + H) |
| 1728        |   | 460 (M + H) |
| 1729        |   | 478 (M + H) |
| 1730        |   | 444 (M + H) |
| 1731        |  | 492 (M + H) |

| Example No. | Structure  | APCI-MS     |
|-------------|--|-------------|
| 1732        |   | 524 (M + H) |
| 1733        |   | 589 (M + H) |
| 1734        |   | 520 (M + H) |
| 1735        |   | 490 (M + H) |
| 1736        |  | 563 (M + H) |

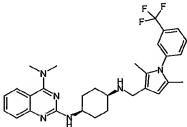
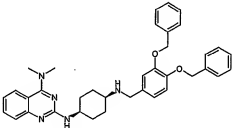
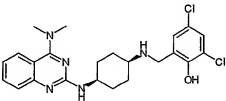
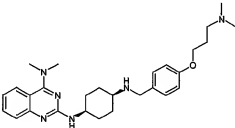
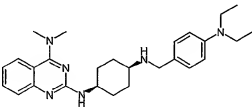
| Example No. | Structure  | APCI-MS     |
|-------------|--|-------------|
| 1737        |   | 471 (M + H) |
| 1738        |   | 578 (M + H) |
| 1739        |   | 410 (M + H) |
| 1740        |   | 424 (M + H) |
| 1741        |  | 424 (M + H) |

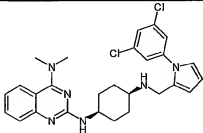
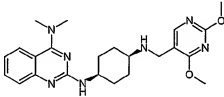
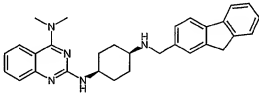
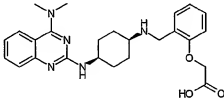
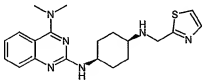
| Example No. | Structure  | APCI-MS      |
|-------------|--|--------------|
| 1742        |   | 424 (M + H)  |
| 1743        |   | 447 (M + Na) |
| 1744        |   | 384 (M + H)  |
| 1745        |   | 424 (M + H)  |
| 1746        |  | 434 (M + H)  |

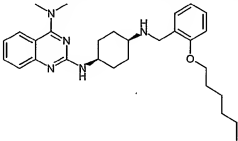
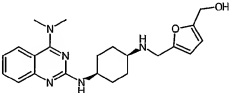
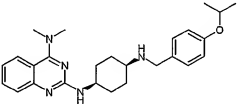
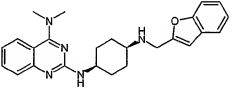
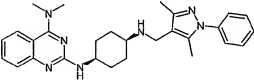
| Example No. | Structure  | APCI-MS     |
|-------------|--|-------------|
| 1747        |   | 472 (M + H) |
| 1748        |   | 520 (M + H) |
| 1749        |   | 514 (M + H) |
| 1750        |   | 470 (M + H) |
| 1751        |  | 500 (M + H) |

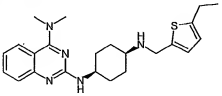
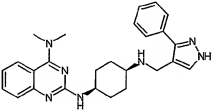
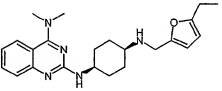
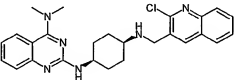
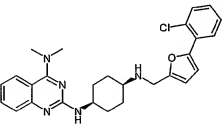
| Example No. | Structure  | APCI-MS     |
|-------------|--|-------------|
| 1752        |   | 482 (M + H) |
| 1753        |   | 502 (M + H) |
| 1754        |   | 490 (M + H) |
| 1755        |   | 426 (M + H) |
| 1756        |  | 683 (M + H) |

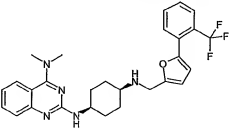
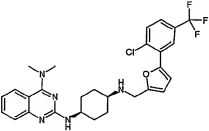
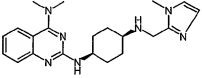
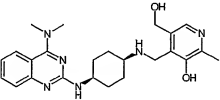
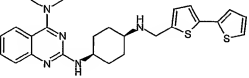


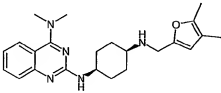
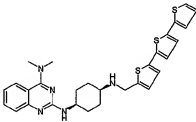
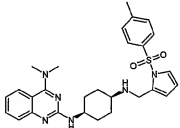
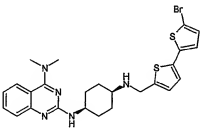
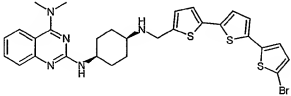
| Example No. | Structure  | APCI-MS     |
|-------------|--|-------------|
| 1757        |   | 537 (M + H) |
| 1758        |   | 588 (M + H) |
| 1759        |   | 460 (M + H) |
| 1760        |   | 477 (M + H) |
| 1761        |  | 447 (M + H) |

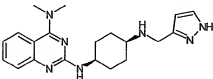
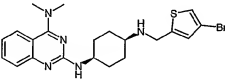
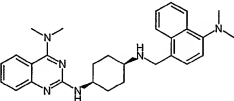
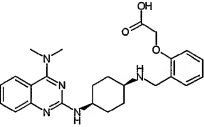
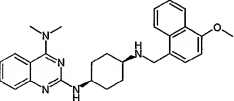
| Example No. | Structure  | APCI-MS     |
|-------------|--|-------------|
| 1762        |   | 509 (M + H) |
| 1763        |   | 438 (M + H) |
| 1764        |   | 464 (M + H) |
| 1765        |   | 450 (M + H) |
| 1766        |  | 383 (M + H) |

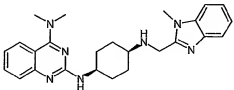
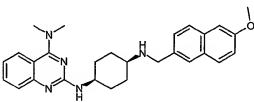
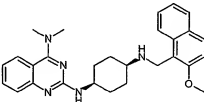
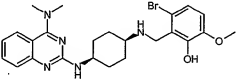
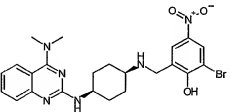
| Example No. | Structure  | APCI-MS     |
|-------------|--|-------------|
| 1767        |   | 476 (M + H) |
| 1768        |   | 396 (M + H) |
| 1769        |   | 434 (M + H) |
| 1770        |   | 416 (M + H) |
| 1771        |  | 470 (M + H) |

| Example No. | Structure  | APCI-MS     |
|-------------|--|-------------|
| 1772        |   | 410 (M + H) |
| 1773        |   | 442 (M + H) |
| 1774        |   | 394 (M + H) |
| 1775        |   | 461 (M + H) |
| 1776        |  | 476 (M + H) |

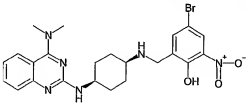
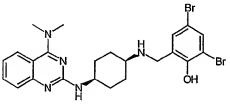
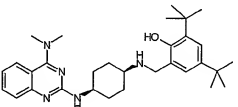
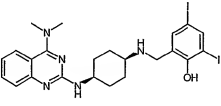
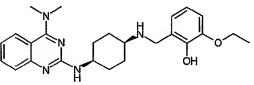
| Example No. | Structure  | APCI-MS     |
|-------------|--|-------------|
| 1777        |   | 510 (M + H) |
| 1778        |   | 544 (M + H) |
| 1779        |   | 380 (M + H) |
| 1780        |   | 437 (M + H) |
| 1781        |  | 464 (M + H) |

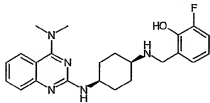
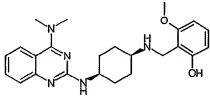
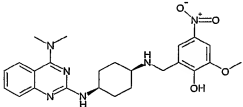
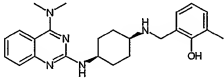
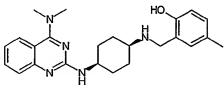
| Example No. | Structure  | APCI-MS     |
|-------------|--|-------------|
| 1782        |   | 394 (M + H) |
| 1783        |   | 546 (M + H) |
| 1784        |   | 519 (M + H) |
| 1785        |   | 542 (M + H) |
| 1786        |  | 624 (M + H) |

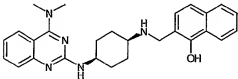
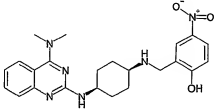
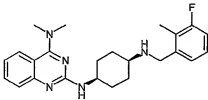
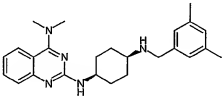
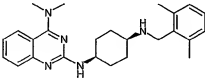
| Example No. | Structure  | APCI-MS     |
|-------------|--|-------------|
| 1787        |   | 366 (M + H) |
| 1788        |   | 460 (M + H) |
| 1789        |   | 469 (M + H) |
| 1790        |   | 450 (M + H) |
| 1791        |  | 456 (M + H) |

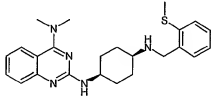
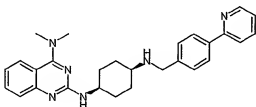
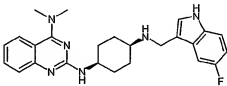
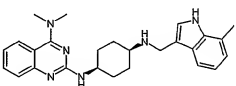
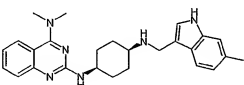
| Example No. | Structure  | APCI-MS      |
|-------------|--|--------------|
| 1792        |   | 430 (M + H)  |
| 1793        |   | 456 (M + H)  |
| 1794        |   | 456 (M + H)  |
| 1795        |   | 500 (M + H)  |
| 1796        |  | 537 (M + Na) |

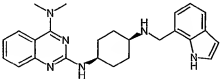
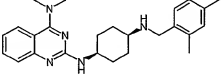
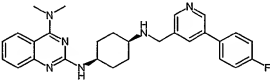
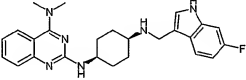
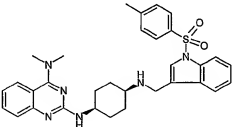


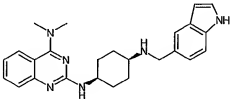
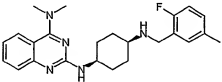
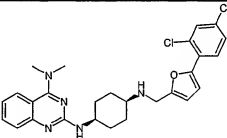
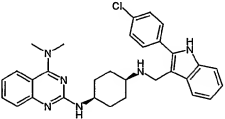
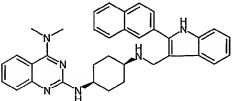
| Example No. | Structure  | APCI-MS      |
|-------------|--|--------------|
| 1797        |   | 537 (M + Na) |
| 1798        |   | 548 (M + H)  |
| 1799        |   | 504 (M + H)  |
| 1800        |   | 644 (M + H)  |
| 1801        |  | 436 (M + H)  |

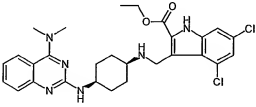
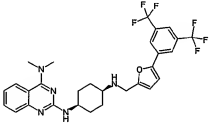
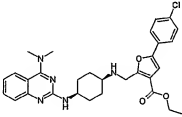
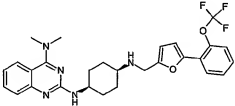
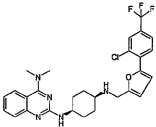
| Example No. | Structure  | APCI-MS     |
|-------------|--|-------------|
| 1802        |   | 410 (M + H) |
| 1803        |   | 422 (M + H) |
| 1804        |   | 467 (M + H) |
| 1805        |   | 406 (M + H) |
| 1806        |  | 406 (M + H) |

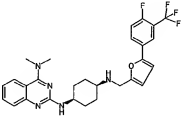
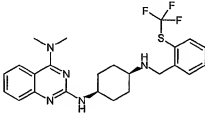
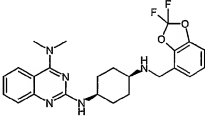
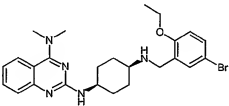
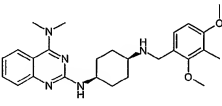
| Example No. | Structure  | APCI-MS     |
|-------------|--|-------------|
| 1807        |   | 440 (M - H) |
| 1808        |   | 437 (M + H) |
| 1809        |   | 408 (M + H) |
| 1810        |   | 404 (M + H) |
| 1811        |  | 404 (M + H) |

| Example No. | Structure  | APCI-MS     |
|-------------|--|-------------|
| 1812        |   | 422 (M + H) |
| 1813        |   | 453 (M + H) |
| 1814        |   | 433 (M + H) |
| 1815        |   | 429 (M + H) |
| 1816        |  | 429 (M + H) |

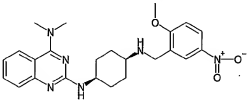
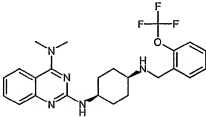
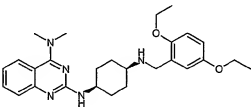
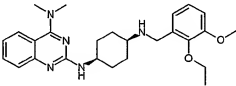
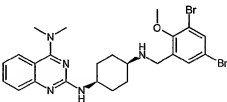
| Example No. | Structure  | APCI-MS     |
|-------------|--|-------------|
| 1817        |   | 415 (M + H) |
| 1818        |   | 404 (M + H) |
| 1819        |   | 471 (M + H) |
| 1820        |   | 433 (M + H) |
| 1821        |  | 569 (M + H) |

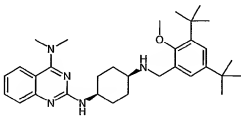
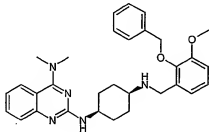
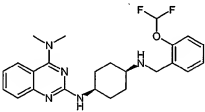
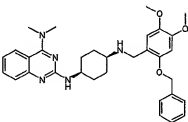
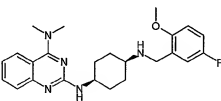
| Example No. | Structure  | APCI-MS     |
|-------------|--|-------------|
| 1822        |   | 415 (M + H) |
| 1823        |   | 408 (M + H) |
| 1824        |   | 510 (M + H) |
| 1825        |   | 525 (M + H) |
| 1826        |  | 541 (M + H) |

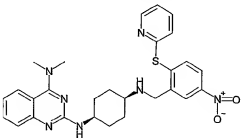
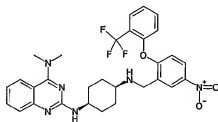
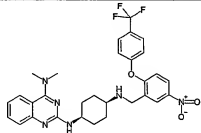
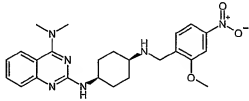
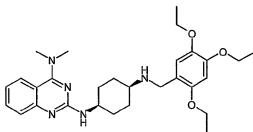
| Example No. | Structure  | APCI-MS     |
|-------------|--|-------------|
| 1827        |   | 555 (M + H) |
| 1828        |   | 578 (M + H) |
| 1829        |   | 548 (M + H) |
| 1830        |   | 526 (M + H) |
| 1831        |  | 544 (M + H) |

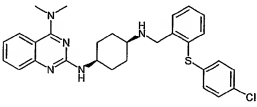
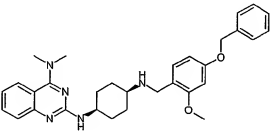
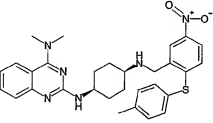
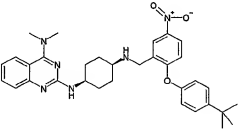
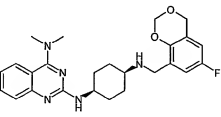
| Example No. | Structure  | APCI-MS     |
|-------------|--|-------------|
| 1832        |   | 528 (M + H) |
| 1833        |   | 476 (M + H) |
| 1834        |   | 456 (M + H) |
| 1835        |   | 498 (M + H) |
| 1836        |  | 450 (M + H) |

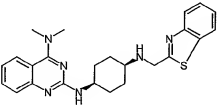
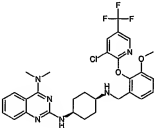
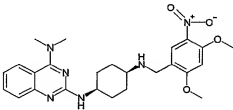
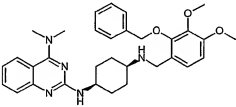
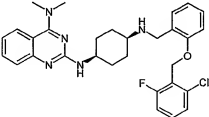


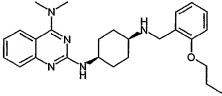
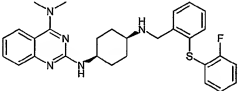
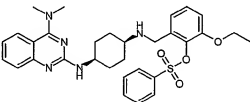
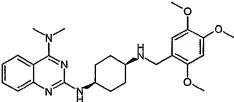
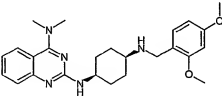
| Example No. | Structure  | APCI-MS     |
|-------------|--|-------------|
| 1837        |   | 451 (M + H) |
| 1838        |   | 460 (M + H) |
| 1839        |   | 464 (M + H) |
| 1840        |   | 450 (M + H) |
| 1841        |  | 562 (M + H) |

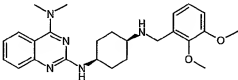
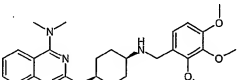
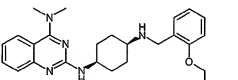
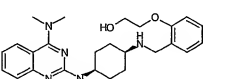
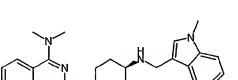
| Example No. | Structure  | APCI-MS     |
|-------------|--|-------------|
| 1842        |   | 518 (M + H) |
| 1843        |   | 512 (M + H) |
| 1844        |   | 442 (M + H) |
| 1845        |   | 542 (M + H) |
| 1846        |  | 424 (M + H) |

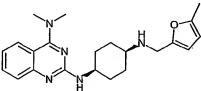
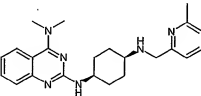
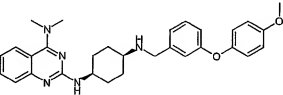
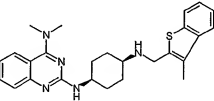
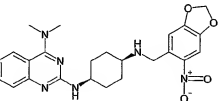
| Example No. | Structure  | APCI-MS     |
|-------------|--|-------------|
| 1847        |   | 530 (M + H) |
| 1848        |   | 581 (M + H) |
| 1849        |   | 581 (M + H) |
| 1850        |   | 451 (M + H) |
| 1851        |  | 508 (M + H) |

| Example No. | Structure  | APCI-MS     |
|-------------|--|-------------|
| 1852        |   | 518 (M + H) |
| 1853        |   | 512 (M + H) |
| 1854        |   | 543 (M + H) |
| 1855        |   | 569 (M + H) |
| 1856        |  | 452 (M + H) |

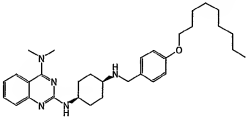
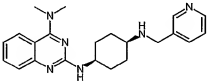
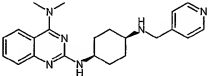
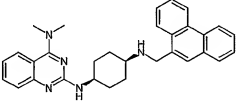
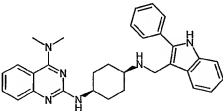
| Example No. | Structure  | APCI-MS     |
|-------------|--|-------------|
| 1857        |   | 433 (M + H) |
| 1858        |   | 601 (M + H) |
| 1859        |   | 481 (M + H) |
| 1860        |   | 542 (M + H) |
| 1861        |  | 534 (M + H) |

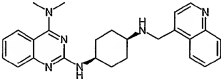
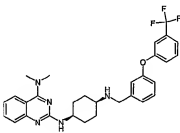
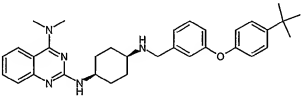
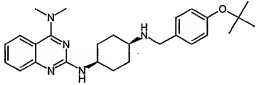
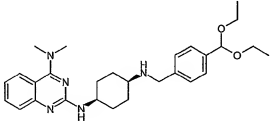
| Example No. | Structure  | APCI-MS     |
|-------------|--|-------------|
| 1862        |   | 434 (M + H) |
| 1863        |   | 502 (M + H) |
| 1864        |   | 576 (M + H) |
| 1865        |   | 466 (M + H) |
| 1866        |  | 436 (M + H) |

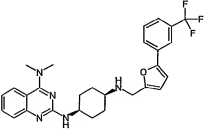
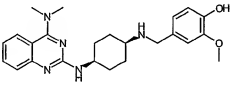
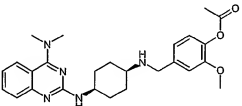
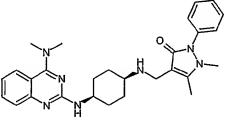
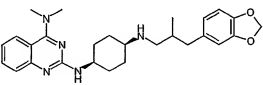
| Example No. | Structure   | APCI-MS     |
|-------------|---|-------------|
| 1867        |  | 436 (M + H) |
| 1868        |  | 466 (M + H) |
| 1869        |  | 432 (M + H) |
| 1870        |  | 436 (M + H) |
| 1871        |  | 429 (M + H) |

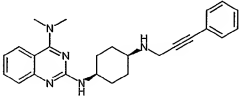
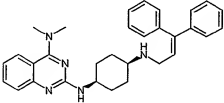
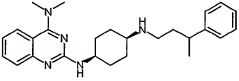
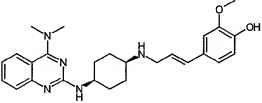
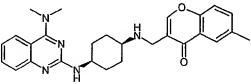
| Example No. | Structure  | APCI-MS     |
|-------------|--|-------------|
| 1872        |   | 380 (M + H) |
| 1873        |   | 391 (M + H) |
| 1874        |   | 498 (M + H) |
| 1875        |   | 446 (M + H) |
| 1876        |  | 465 (M + H) |

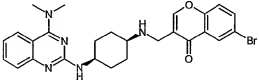
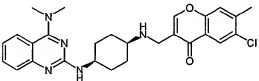
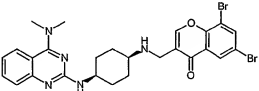
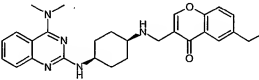
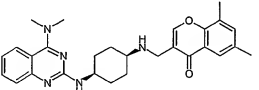


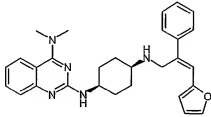
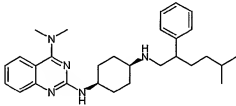
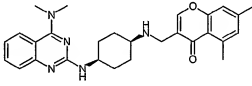
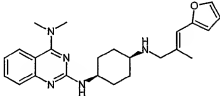
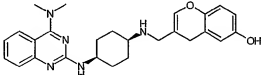
| Example No. | Structure  | APCI-MS     |
|-------------|--|-------------|
| 1877        |   | 518 (M + H) |
| 1878        |   | 377 (M + H) |
| 1879        |   | 377 (M + H) |
| 1880        |   | 476 (M + H) |
| 1881        |  | 491 (M + H) |

| Example No. | Structure  | APCI-MS     |
|-------------|--|-------------|
| 1882        |   | 427 (M + H) |
| 1883        |   | 536 (M + H) |
| 1884        |   | 524 (M + H) |
| 1885        |   | 448 (M + H) |
| 1886        |  | 478 (M + H) |

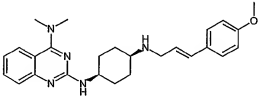
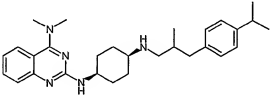
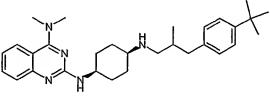
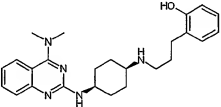
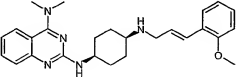
| Example No. | Structure  | APCI-MS     |
|-------------|--|-------------|
| 1887        |   | 510 (M + H) |
| 1888        |   | 422 (M + H) |
| 1889        |   | 464 (M + H) |
| 1890        |   | 486 (M + H) |
| 1891        |  | 462 (M + H) |

| Example No. | Structure  | APCI-MS     |
|-------------|--|-------------|
| 1892        |   | 400 (M + H) |
| 1893        |   | 478 (M + H) |
| 1894        |   | 418 (M + H) |
| 1895        |   | 448 (M + H) |
| 1896        |  | 458 (M + H) |

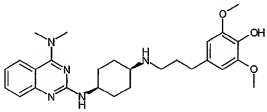
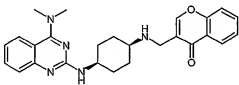
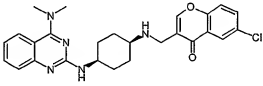
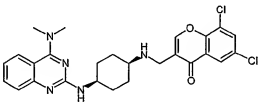
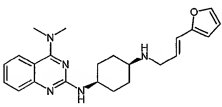
| Example No. | Structure  | APCI-MS     |
|-------------|--|-------------|
| 1897        |   | 522 (M + H) |
| 1898        |   | 492 (M + H) |
| 1899        |   | 600 (M + H) |
| 1900        |   | 472 (M + H) |
| 1901        |  | 472 (M + H) |

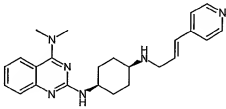
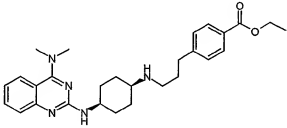
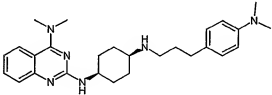
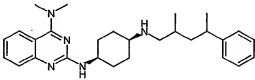
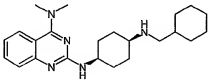
| Example No. | Structure  | APCI-MS     |
|-------------|--|-------------|
| 1902        |   | 468 (M + H) |
| 1903        |   | 460 (M + H) |
| 1904        |   | 472 (M + H) |
| 1905        |   | 406 (M + H) |
| 1906        |  | 446 (M + H) |

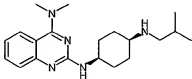
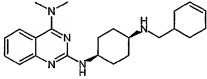
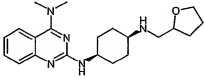
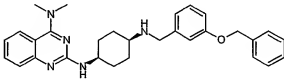
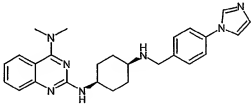


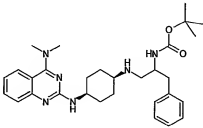
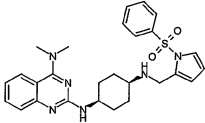
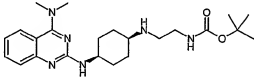
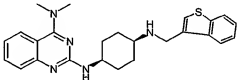
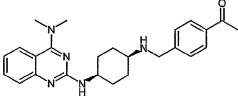
| Example No. | Structure  | APCI-MS     |
|-------------|--|-------------|
| 1912        |   | 432 (M + H) |
| 1913        |   | 460 (M + H) |
| 1914        |   | 474 (M + H) |
| 1915        |   | 420 (M + H) |
| 1916        |  | 432 (M + H) |

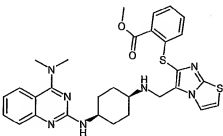
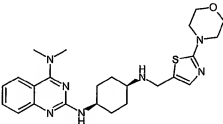
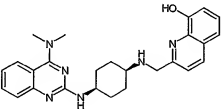
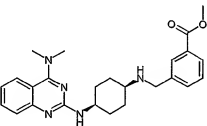
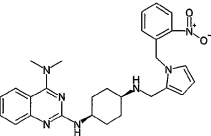


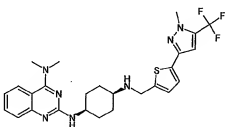
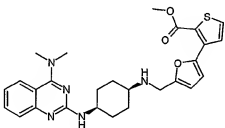
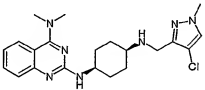
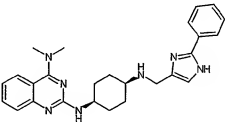
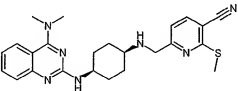
| Example No. | Structure  | APCI-MS     |
|-------------|--|-------------|
| 1917        |   | 480 (M + H) |
| 1918        |   | 444 (M + H) |
| 1919        |   | 478 (M + H) |
| 1920        |   | 512 (M + H) |
| 1921        |  | 392 (M + H) |

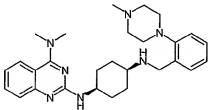
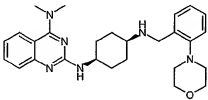
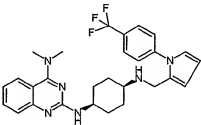
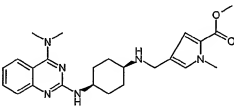
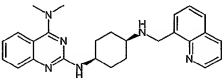
| Example No. | Structure  | APCI-MS     |
|-------------|--|-------------|
| 1922        |   | 403 (M + H) |
| 1923        |   | 476 (M + H) |
| 1924        |   | 447 (M + H) |
| 1925        |   | 446 (M + H) |
| 1926        |  | 382 (M + H) |

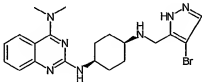
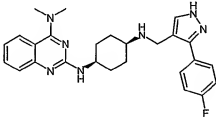
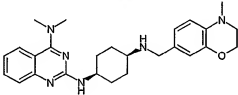
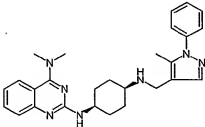
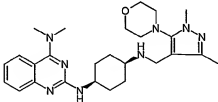
| Example No. | Structure  | APCI-MS     |
|-------------|--|-------------|
| 1927        |   | 342 (M + H) |
| 1928        |   | 380 (M + H) |
| 1929        |   | 370 (M + H) |
| 1930        |   | 482 (M + H) |
| 1931        |  | 442 (M + H) |

| Example No. | Structure  | APCI-MS     |
|-------------|--|-------------|
| 1932        |   | 519 (M + H) |
| 1933        |   | 505 (M + H) |
| 1934        |   | 429 (M + H) |
| 1935        |   | 432 (M + H) |
| 1936        |  | 418 (M + H) |

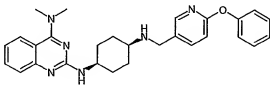
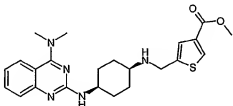
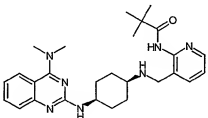
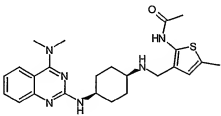
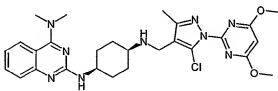
| Example No. | Structure  | APCI-MS     |
|-------------|--|-------------|
| 1937        |   | 588 (M + H) |
| 1938        |   | 468 (M + H) |
| 1939        |   | 443 (M + H) |
| 1940        |   | 434 (M + H) |
| 1941        |  | 500 (M + H) |

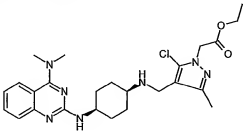
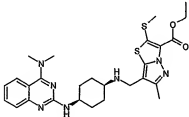
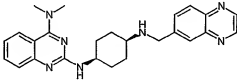
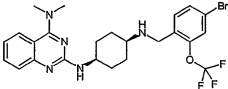
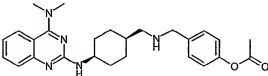
| Example No. | Structure  | APCI-MS     |
|-------------|--|-------------|
| 1942        |   | 530 (M + H) |
| 1943        |   | 506 (M + H) |
| 1944        |   | 414 (M + H) |
| 1945        |   | 442 (M + H) |
| 1946        |  | 448 (M + H) |

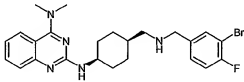
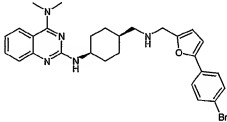
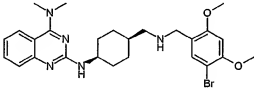
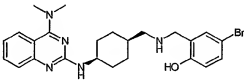
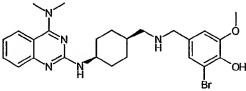
| Example No. | Structure  | APCI-MS     |
|-------------|--|-------------|
| 1947        |   | 474 (M + H) |
| 1948        |   | 461 (M + H) |
| 1949        |   | 509 (M + H) |
| 1950        |   | 437 (M + H) |
| 1951        |  | 427 (M + H) |

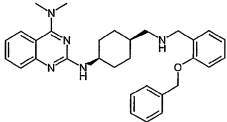
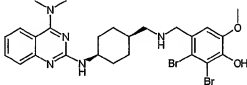
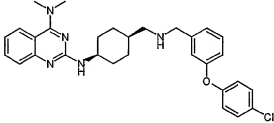
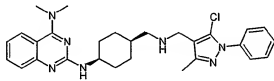
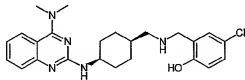
| Example No. | Structure  | APCI-MS     |
|-------------|--|-------------|
| 1952        |   | 444 (M + H) |
| 1953        |   | 460 (M + H) |
| 1954        |   | 447 (M + H) |
| 1955        |   | 456 (M + H) |
| 1956        |  | 479 (M + H) |



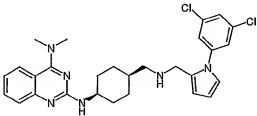
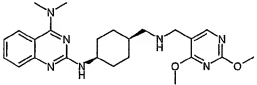
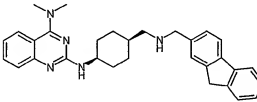
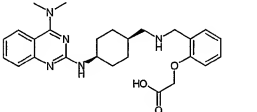
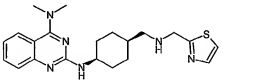
| Example No. | Structure  | APCI-MS     |
|-------------|--|-------------|
| 1957        |   | 469 (M + H) |
| 1958        |   | 440 (M + H) |
| 1959        |   | 476 (M + H) |
| 1960        |   | 453 (M + H) |
| 1961        |  | 552 (M + H) |

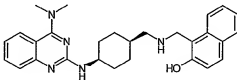
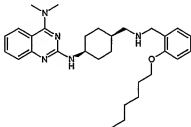
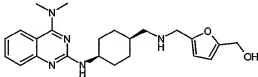
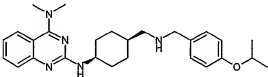
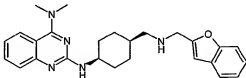
| Example No. | Structure  | APCI-MS     |
|-------------|--|-------------|
| 1962        |   | 500 (M + H) |
| 1963        |   | 554 (M + H) |
| 1964        |   | 428 (M + H) |
| 1965        |   | 538 (M + H) |
| 1966        |  | 448 (M + H) |

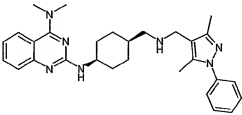
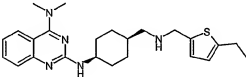
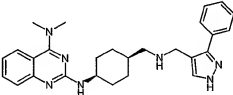
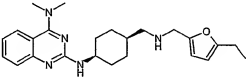
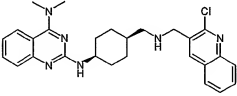
| Example No. | Structure  | APCI-MS     |
|-------------|--|-------------|
| 1967        |   | 486 (M + H) |
| 1968        |   | 534 (M + H) |
| 1969        |   | 528 (M + H) |
| 1970        |   | 484 (M + H) |
| 1971        |  | 514 (M + H) |

| Example No. | Structure  | APCI-MS     |
|-------------|--|-------------|
| 1972        |   | 496 (M + H) |
| 1973        |   | 592 (M + H) |
| 1974        |   | 516 (M + H) |
| 1975        |   | 504 (M + H) |
| 1976        |  | 440 (M + H) |

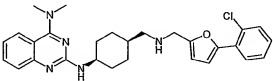
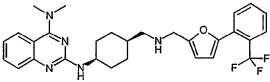
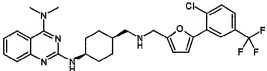
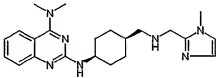
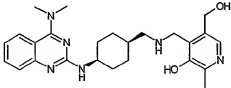
| Example No. | Structure | APCI-MS     |
|-------------|-----------|-------------|
| 1977        |           | 697 (M + H) |
| 1978        |           | 551 (M + H) |
| 1979        |           | 602 (M + H) |
| 1980        |           | 474 (M + H) |
| 1981        |           | 491 (M + H) |

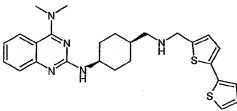
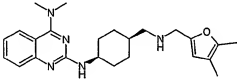
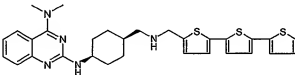
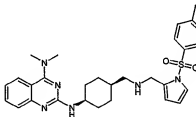
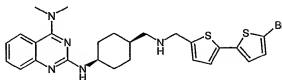
| Example No. | Structure  | APCI-MS     |
|-------------|--|-------------|
| 1982        |   | 523 (M + H) |
| 1983        |   | 452 (M + H) |
| 1984        |   | 478 (M + H) |
| 1985        |   | 464 (M + H) |
| 1986        |  | 397 (M + H) |

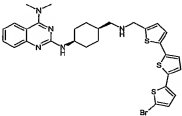
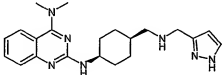
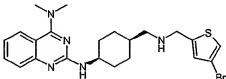
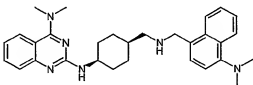
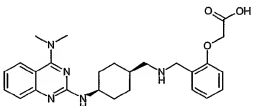
| Example No. | Structure  | APCI-MS     |
|-------------|--|-------------|
| 1987        |   | 454 (M - H) |
| 1988        |   | 490 (M + H) |
| 1989        |   | 410 (M + H) |
| 1990        |   | 448 (M + H) |
| 1991        |  | 430 (M + H) |

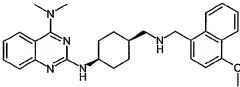
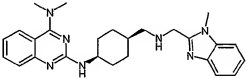
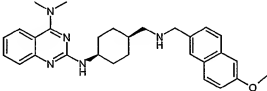
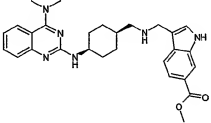
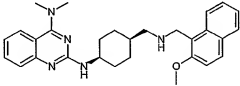
| Example No. | Structure  | APCI-MS     |
|-------------|--|-------------|
| 1992        |   | 484 (M + H) |
| 1993        |   | 424 (M + H) |
| 1994        |   | 456 (M + H) |
| 1995        |   | 408 (M + H) |
| 1996        |  | 475 (M + H) |

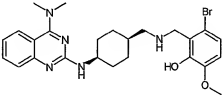
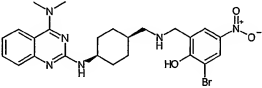
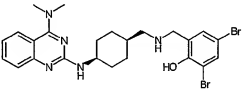
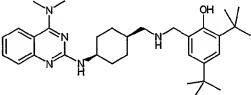
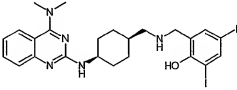


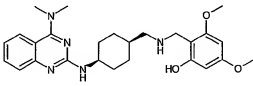
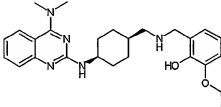
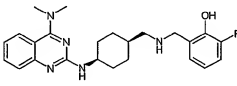
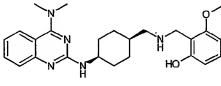
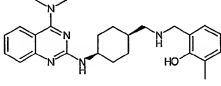
| Example No. | Structure  | APCI-MS     |
|-------------|--|-------------|
| 1997        |   | 490 (M + H) |
| 1998        |   | 524 (M + H) |
| 1999        |   | 558 (M + H) |
| 2000        |   | 394 (M + H) |
| 2001        |  | 451 (M + H) |

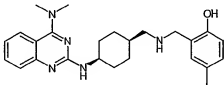
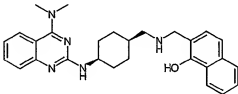
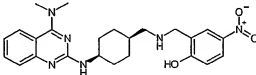
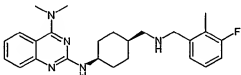
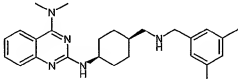
| Example No. | Structure  | APCI-MS     |
|-------------|--|-------------|
| 2002        |   | 478 (M + H) |
| 2003        |   | 408 (M + H) |
| 2004        |   | 560 (M + H) |
| 2005        |   | 533 (M + H) |
| 2006        |  | 556 (M + H) |

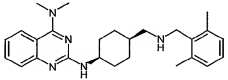
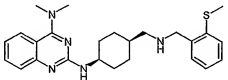
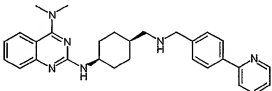
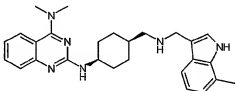
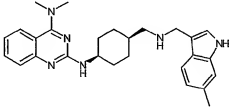
| Example No. | Structure  | APCI-MS     |
|-------------|--|-------------|
| 2007        |   | 638 (M + H) |
| 2008        |   | 380 (M + H) |
| 2009        |   | 474 (M + H) |
| 2010        |   | 483 (M + H) |
| 2011        |  | 464 (M + H) |

| Example No. | Structure  | APCI-MS     |
|-------------|--|-------------|
| 2012        |   | 470 (M + H) |
| 2013        |   | 444 (M + H) |
| 2014        |   | 470 (M + H) |
| 2015        |   | 487 (M + H) |
| 2016        |  | 470 (M + H) |

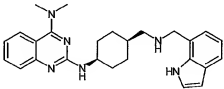
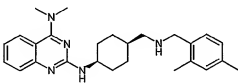
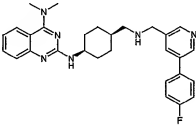
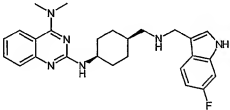
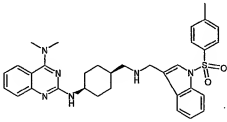
| Example No. | Structure  | APCI-MS     |
|-------------|--|-------------|
| 2017        |   | 514 (M + H) |
| 2018        |   | 527 (M - H) |
| 2019        |   | 562 (M + H) |
| 2020        |   | 518 (M + H) |
| 2021        |  | 658 (M + H) |

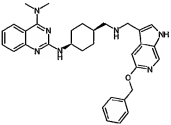
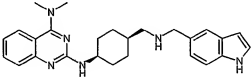
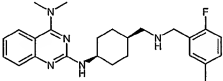
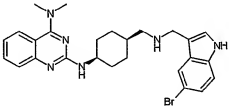
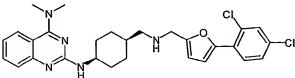
| Example No. | Structure  | APCI-MS     |
|-------------|--|-------------|
| 2022        |   | 466 (M + H) |
| 2023        |   | 450 (M + H) |
| 2024        |   | 424 (M + H) |
| 2025        |   | 436 (M + H) |
| 2026        |  | 420 (M + H) |

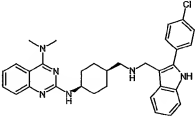
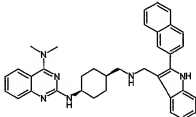
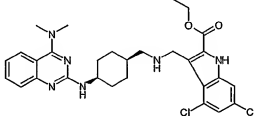
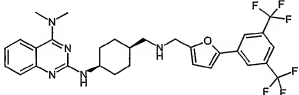
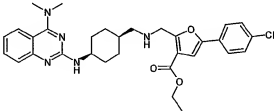
| Example No. | Structure  | APCI-MS     |
|-------------|--|-------------|
| 2027        |   | 420 (M + H) |
| 2028        |   | 456 (M + H) |
| 2029        |   | 451 (M + H) |
| 2030        |   | 422 (M + H) |
| 2031        |  | 418 (M + H) |

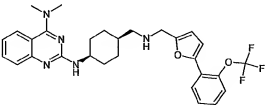
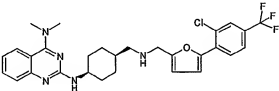
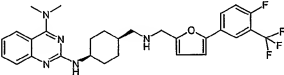
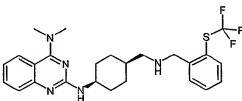
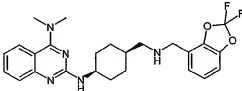
| Example No. | Structure  | APCI-MS     |
|-------------|--|-------------|
| 2032        |   | 418 (M + H) |
| 2033        |   | 436 (M + H) |
| 2034        |   | 467 (M + H) |
| 2035        |   | 443 (M + H) |
| 2036        |  | 443 (M + H) |

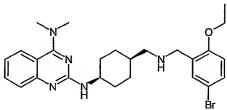
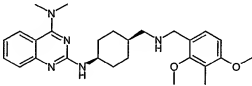
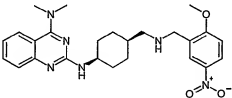
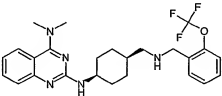
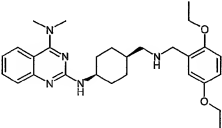


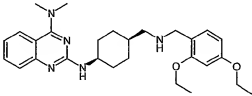
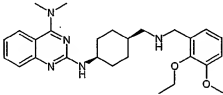
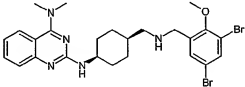
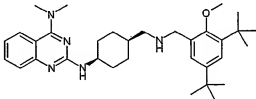
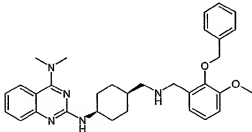
| Example No. | Structure  | APCI-MS     |
|-------------|--|-------------|
| 2037        |   | 429 (M + H) |
| 2038        |   | 418 (M + H) |
| 2039        |   | 485 (M + H) |
| 2040        |   | 447 (M + H) |
| 2041        |  | 583 (M + H) |

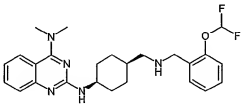
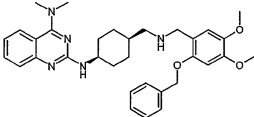
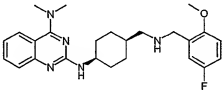
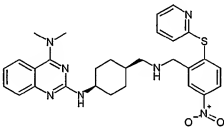
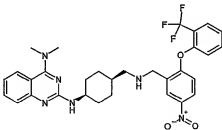
| Example No. | Structure  | APCI-MS     |
|-------------|--|-------------|
| 2042        |   | 536 (M + H) |
| 2043        |   | 429 (M + H) |
| 2044        |   | 422 (M + H) |
| 2045        |   | 507 (M + H) |
| 2046        |  | 524 (M + H) |

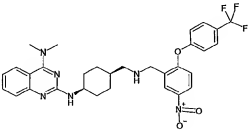
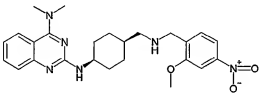
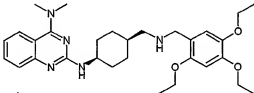
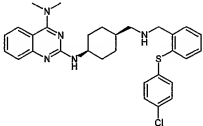
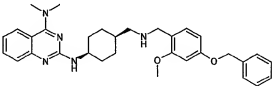
| Example No. | Structure  | APCI-MS     |
|-------------|--|-------------|
| 2047        |   | 539 (M + H) |
| 2048        |   | 555 (M + H) |
| 2049        |   | 569 (M + H) |
| 2050        |   | 592 (M + H) |
| 2051        |  | 562 (M + H) |

| Example No. | Structure  | APCI-MS     |
|-------------|--|-------------|
| 2052        |   | 540 (M + H) |
| 2053        |   | 558 (M + H) |
| 2054        |   | 542 (M + H) |
| 2055        |   | 490 (M + H) |
| 2056        |  | 470 (M + H) |

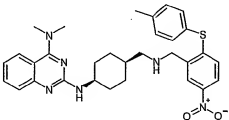
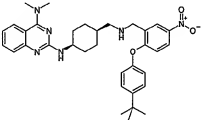
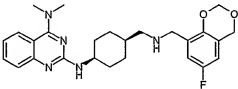
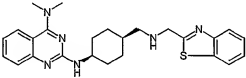
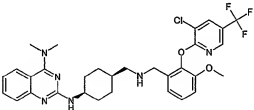
| Example No. | Structure  | APCI-MS     |
|-------------|--|-------------|
| 2057        |   | 512 (M + H) |
| 2058        |   | 464 (M + H) |
| 2059        |   | 465 (M + H) |
| 2060        |   | 474 (M + H) |
| 2061        |  | 478 (M + H) |

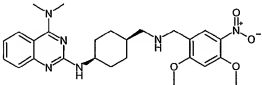
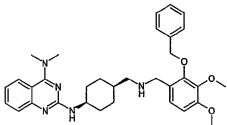
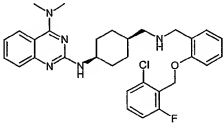
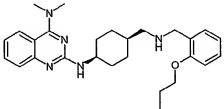
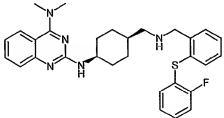
| Example No. | Structure  | APCI-MS     |
|-------------|--|-------------|
| 2062        |   | 478 (M + H) |
| 2063        |   | 464 (M + H) |
| 2064        |   | 576 (M + H) |
| 2065        |   | 532 (M + H) |
| 2066        |  | 526 (M + H) |

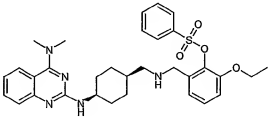
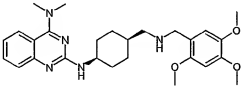
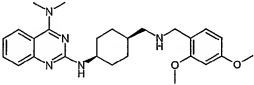
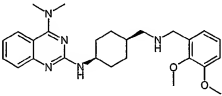
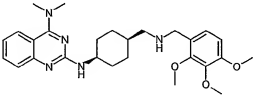
| Example No. | Structure  | APCI-MS     |
|-------------|--|-------------|
| 2067        |   | 456 (M + H) |
| 2068        |   | 556 (M + H) |
| 2069        |   | 438 (M + H) |
| 2070        |   | 544 (M + H) |
| 2071        |  | 595 (M + H) |

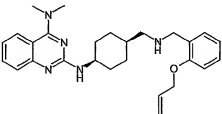
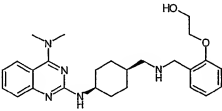
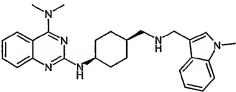
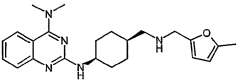
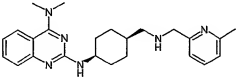
| Example No. | Structure  | APCI-MS     |
|-------------|--|-------------|
| 2072        |   | 595 (M + H) |
| 2073        |   | 465 (M + H) |
| 2074        |   | 522 (M + H) |
| 2075        |   | 532 (M + H) |
| 2076        |  | 526 (M + H) |

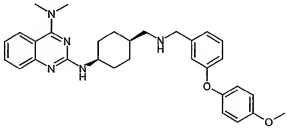
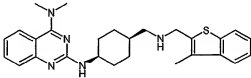
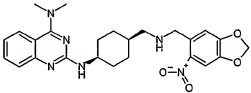
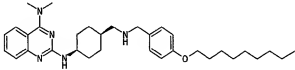
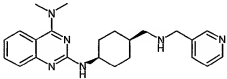


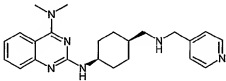
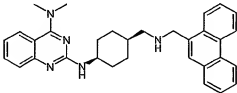
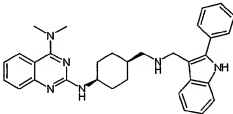
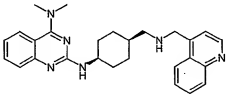
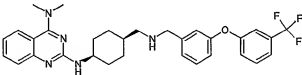
| Example No. | Structure  | APCI-MS     |
|-------------|--|-------------|
| 2077        |   | 557 (M + H) |
| 2078        |   | 583 (M + H) |
| 2079        |   | 466 (M + H) |
| 2080        |   | 447 (M + H) |
| 2081        |  | 615 (M + H) |

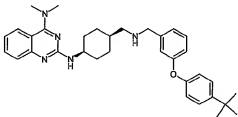
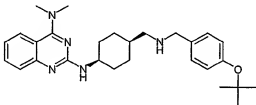
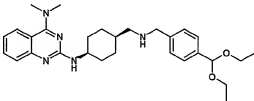
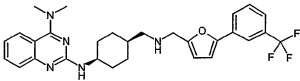
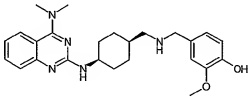
| Example No. | Structure  | APCI-MS     |
|-------------|--|-------------|
| 2082        |   | 495 (M + H) |
| 2083        |   | 556 (M + H) |
| 2084        |   | 548 (M + H) |
| 2085        |   | 448 (M + H) |
| 2086        |  | 516 (M + H) |

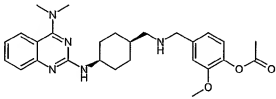
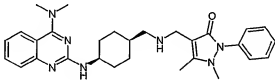
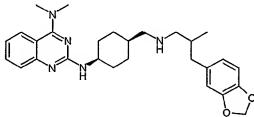
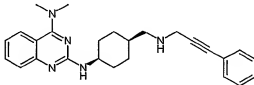
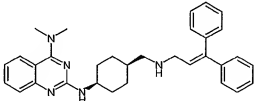
| Example No. | Structure  | APCI-MS     |
|-------------|--|-------------|
| 2087        |   | 590 (M + H) |
| 2088        |   | 480 (M + H) |
| 2089        |   | 450 (M + H) |
| 2090        |   | 450 (M + H) |
| 2091        |  | 480 (M + H) |

| Example No. | Structure  | APCI-MS     |
|-------------|--|-------------|
| 2092        |   | 446 (M + H) |
| 2093        |   | 450 (M + H) |
| 2094        |   | 443 (M + H) |
| 2095        |   | 394 (M + H) |
| 2096        |  | 405 (M + H) |

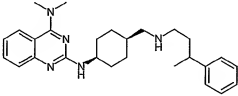
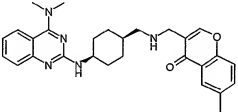
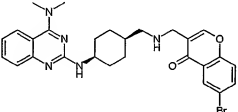
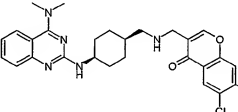
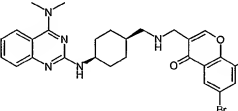
| Example No. | Structure  | APCI-MS     |
|-------------|--|-------------|
| 2097        |   | 512 (M + H) |
| 2098        |   | 460 (M + H) |
| 2099        |   | 479 (M + H) |
| 2100        |   | 532 (M + H) |
| 2101        |  | 391 (M + H) |

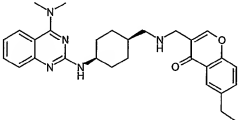
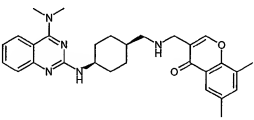
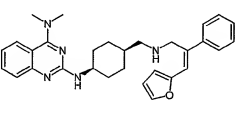
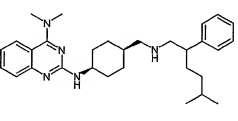
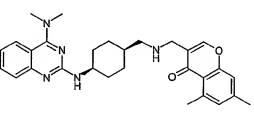
| Example No. | Structure  | APCI-MS     |
|-------------|--|-------------|
| 2102        |   | 391 (M + H) |
| 2103        |   | 490 (M + H) |
| 2104        |   | 505 (M + H) |
| 2105        |   | 441 (M + H) |
| 2106        |  | 550 (M + H) |

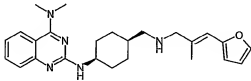
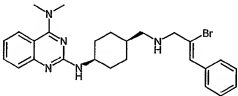
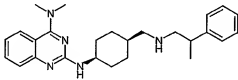
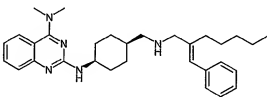
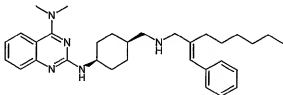
| Example No. | Structure  | APCI-MS     |
|-------------|--|-------------|
| 2107        |   | 538 (M + H) |
| 2108        |   | 462 (M + H) |
| 2109        |   | 492 (M + H) |
| 2110        |   | 524 (M + H) |
| 2111        |  | 436 (M + H) |

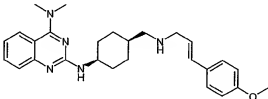
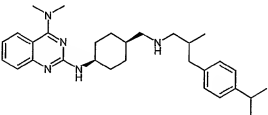
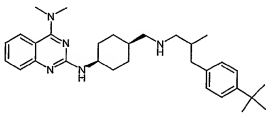
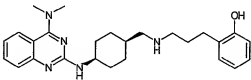
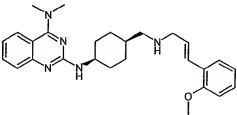
| Example No. | Structure  | APCI-MS     |
|-------------|--|-------------|
| 2112        |   | 478 (M + H) |
| 2113        |   | 500 (M + H) |
| 2114        |   | 476 (M + H) |
| 2115        |   | 414 (M + H) |
| 2116        |  | 492 (M + H) |

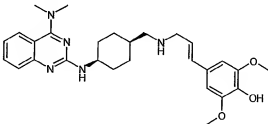
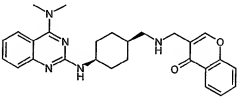
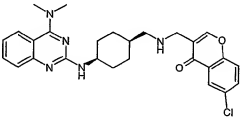
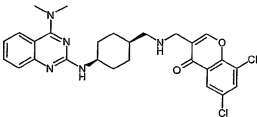
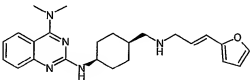


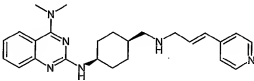
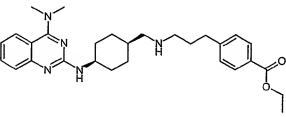
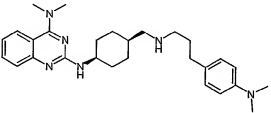
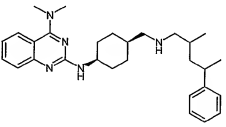
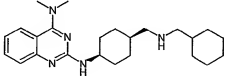
| Example No. | Structure  | APCI-MS     |
|-------------|--|-------------|
| 2117        |   | 432 (M + H) |
| 2118        |   | 472 (M + H) |
| 2119        |   | 536 (M + H) |
| 2120        |   | 506 (M + H) |
| 2121        |  | 614 (M + H) |

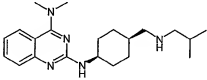
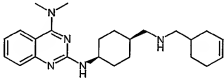
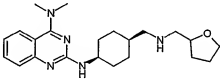
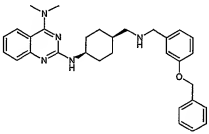
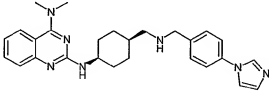
| Example No. | Structure  | APCI-MS     |
|-------------|--|-------------|
| 2122        |   | 486 (M + H) |
| 2123        |   | 486 (M + H) |
| 2124        |   | 482 (M + H) |
| 2125        |   | 474 (M + H) |
| 2126        |  | 486 (M + H) |

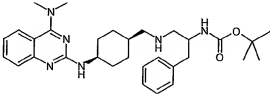
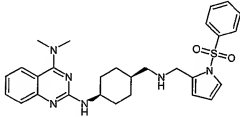
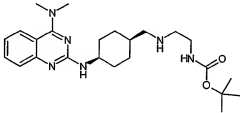
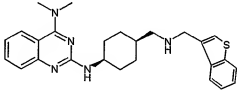
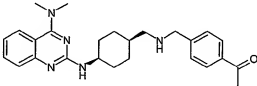
| Example No. | Structure  | APCI-MS     |
|-------------|--|-------------|
| 2127        |   | 420 (M + H) |
| 2128        |   | 494 (M + H) |
| 2129        |   | 418 (M + H) |
| 2130        |   | 486 (M + H) |
| 2131        |  | 500 (M + H) |

| Example No. | Structure  | APCI-MS     |
|-------------|--|-------------|
| 2132        |   | 446 (M + H) |
| 2133        |   | 474 (M + H) |
| 2134        |   | 488 (M + H) |
| 2135        |   | 434 (M + H) |
| 2136        |  | 446 (M + H) |

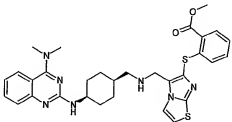
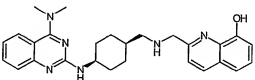
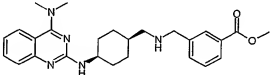
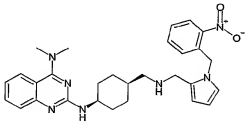
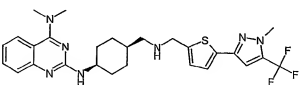
| Example No. | Structure  | APCI-MS     |
|-------------|--|-------------|
| 2137        |   | 492 (M + H) |
| 2138        |   | 458 (M + H) |
| 2139        |   | 492 (M + H) |
| 2140        |   | 526 (M + H) |
| 2141        |  | 406 (M + H) |

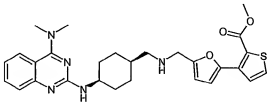
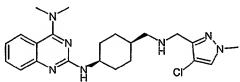
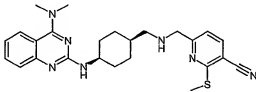
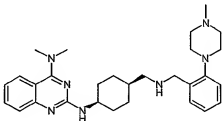
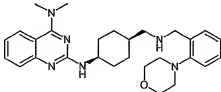
| Example No. | Structure  | APCI-MS     |
|-------------|--|-------------|
| 2142        |   | 417 (M + H) |
| 2143        |   | 490 (M + H) |
| 2144        |   | 461 (M + H) |
| 2145        |   | 460 (M + H) |
| 2146        |  | 396 (M + H) |

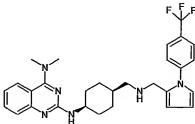
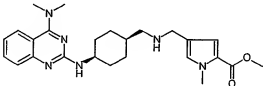
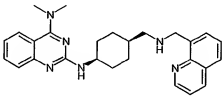
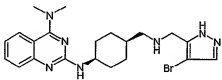
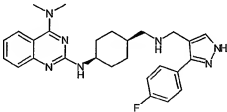
| Example No. | Structure  | APCI-MS     |
|-------------|--|-------------|
| 2147        |   | 356 (M + H) |
| 2148        |   | 394 (M + H) |
| 2149        |   | 384 (M + H) |
| 2150        |   | 496 (M + H) |
| 2151        |  | 456 (M + H) |

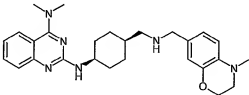
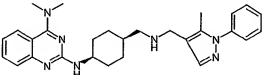
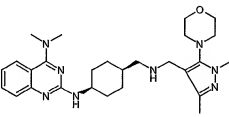
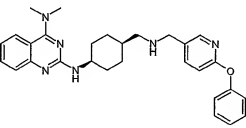
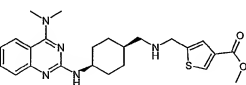
| Example No. | Structure  | APCI-MS     |
|-------------|--|-------------|
| 2152        |   | 533 (M + H) |
| 2153        |   | 519 (M + H) |
| 2154        |   | 443 (M + H) |
| 2155        |   | 446 (M + H) |
| 2156        |  | 432 (M + H) |

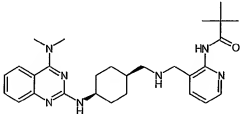
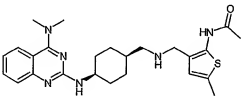
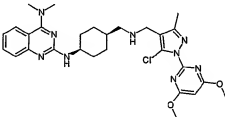
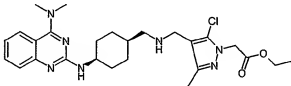
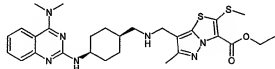


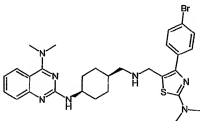
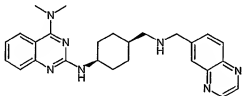
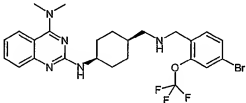
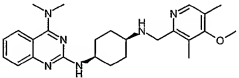
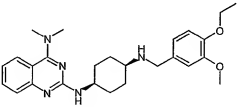
| Example No. | Structure  | APCI-MS     |
|-------------|--|-------------|
| 2157        |   | 602 (M + H) |
| 2158        |   | 457 (M + H) |
| 2159        |   | 448 (M + H) |
| 2160        |   | 514 (M + H) |
| 2161        |  | 544 (M + H) |

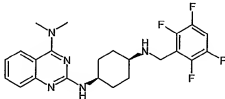
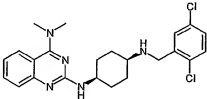
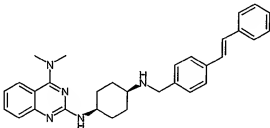
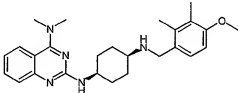
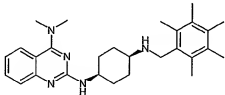
| Example No. | Structure  | APCI-MS     |
|-------------|--|-------------|
| 2162        |   | 520 (M + H) |
| 2163        |   | 428 (M + H) |
| 2164        |   | 462 (M + H) |
| 2165        |   | 488 (M + H) |
| 2166        |  | 475 (M + H) |

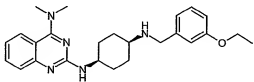
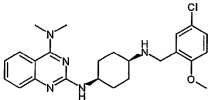
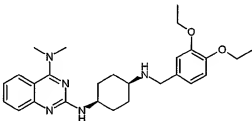
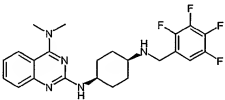
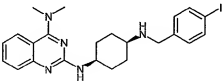
| Example No. | Structure  | APCI-MS     |
|-------------|--|-------------|
| 2167        |   | 523 (M + H) |
| 2168        |   | 451 (M + H) |
| 2169        |   | 441 (M + H) |
| 2170        |   | 458 (M + H) |
| 2171        |  | 474 (M + H) |

| Example No. | Structure  | APCI-MS     |
|-------------|--|-------------|
| 2172        |   | 461 (M + H) |
| 2173        |   | 470 (M + H) |
| 2174        |   | 493 (M + H) |
| 2175        |   | 483 (M + H) |
| 2176        |  | 454 (M + H) |

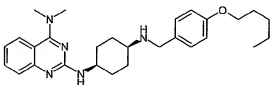
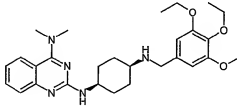
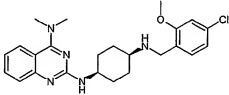
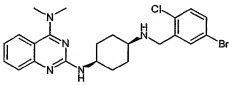
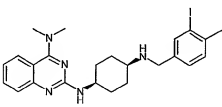
| Example No. | Structure  | APCI-MS     |
|-------------|--|-------------|
| 2177        |   | 490 (M + H) |
| 2178        |   | 467 (M + H) |
| 2179        |   | 566 (M + H) |
| 2180        |   | 514 (M + H) |
| 2181        |  | 568 (M + H) |

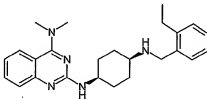
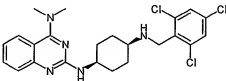
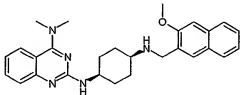
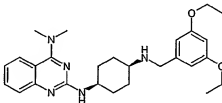
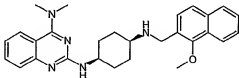
| Example No. | Structure  | APCI-MS     |
|-------------|--|-------------|
| 2182        |   | 594 (M + H) |
| 2183        |   | 442 (M + H) |
| 2184        |   | 552 (M + H) |
| 2185        |   | 435 (M + H) |
| 2186        |  | 450 (M + H) |

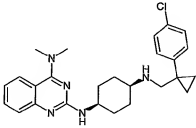
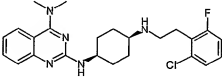
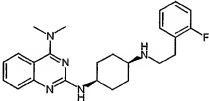
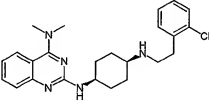
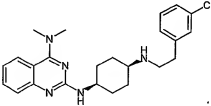
| Example No. | Structure  | APCI-MS     |
|-------------|--|-------------|
| 2187        |   | 448 (M + H) |
| 2188        |   | 444 (M + H) |
| 2189        |   | 478 (M + H) |
| 2190        |   | 434 (M + H) |
| 2191        |  | 446 (M + H) |

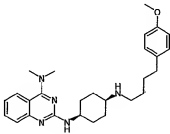
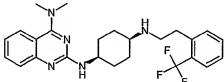
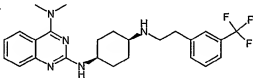
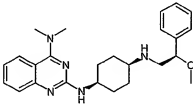
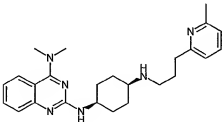
| Example No. | Structure  | APCI-MS     |
|-------------|--|-------------|
| 2192        |   | 420 (M + H) |
| 2193        |   | 440 (M + H) |
| 2194        |   | 464 (M + H) |
| 2195        |   | 448 (M + H) |
| 2196        |  | 502 (M + H) |

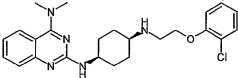
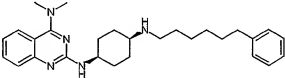
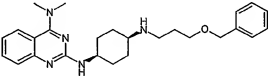
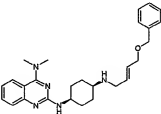
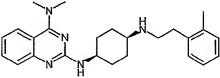


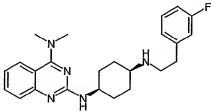
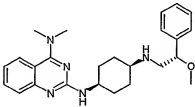
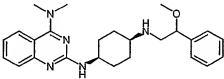
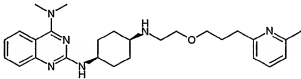
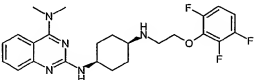
| Example No. | Structure  | APCI-MS     |
|-------------|--|-------------|
| 2197        |   | 462 (M + H) |
| 2198        |   | 508 (M + H) |
| 2199        |   | 440 (M + H) |
| 2200        |   | 488 (M + H) |
| 2201        |  | 516 (M + H) |

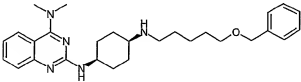
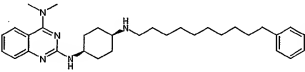
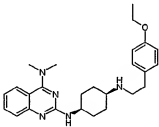
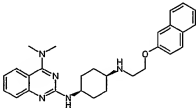
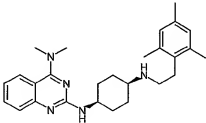
| Example No. | Structure  | APCI-MS     |
|-------------|--|-------------|
| 2202        |   | 404 (M + H) |
| 2203        |   | 478 (M + H) |
| 2204        |   | 456 (M + H) |
| 2205        |   | 464 (M + H) |
| 2206        |  | 456 (M + H) |

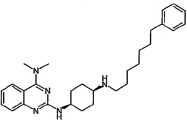
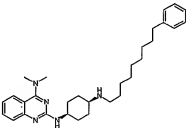
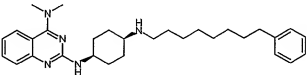
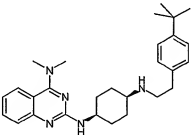
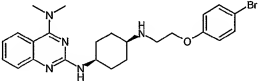
| Example No. | Structure  | APCI-MS     |
|-------------|--|-------------|
| 2207        |   | 450 (M + H) |
| 2208        |   | 442 (M + H) |
| 2209        |   | 408 (M + H) |
| 2210        |   | 424 (M + H) |
| 2211        |  | 424 (M + H) |

| Example No. | Structure  | APCI-MS     |
|-------------|--|-------------|
| 2212        |   | 448 (M + H) |
| 2213        |   | 458 (M + H) |
| 2214        |   | 458 (M + H) |
| 2215        |   | 420 (M + H) |
| 2216        |  | 419 (M + H) |

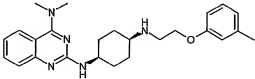
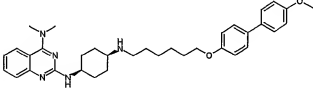
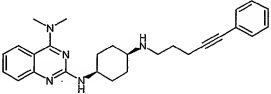
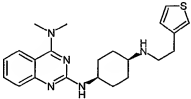
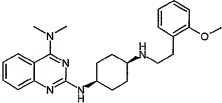
| Example No. | Structure  | APCI-MS     |
|-------------|--|-------------|
| 2217        |   | 440 (M + H) |
| 2218        |   | 446 (M + H) |
| 2219        |   | 434 (M + H) |
| 2220        |   | 446 (M + H) |
| 2221        |  | 404 (M + H) |

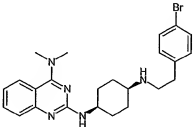
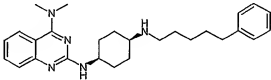
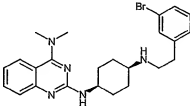
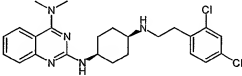
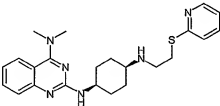
| Example No. | Structure  | APCI-MS     |
|-------------|--|-------------|
| 2222        |   | 408 (M + H) |
| 2223        |   | 420 (M + H) |
| 2224        |   | 420 (M + H) |
| 2225        |   | 463 (M + H) |
| 2226        |  | 460 (M + H) |

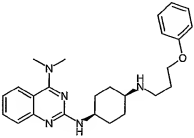
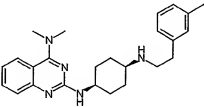
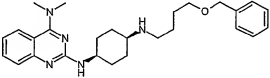
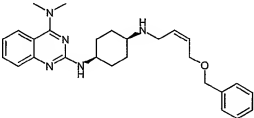
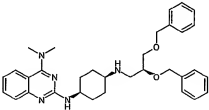
| Example No. | Structure  | APCI-MS     |
|-------------|--|-------------|
| 2227        |   | 462 (M + H) |
| 2228        |   | 502 (M + H) |
| 2229        |   | 434 (M + H) |
| 2230        |   | 456 (M + H) |
| 2231        |  | 432 (M + H) |

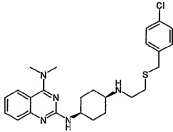
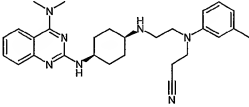
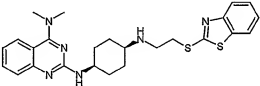
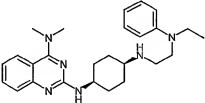
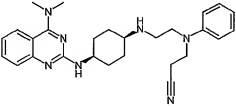
| Example No. | Structure  | APCI-MS     |
|-------------|--|-------------|
| 2232        |   | 460 (M + H) |
| 2233        |   | 488 (M + H) |
| 2234        |   | 474 (M + H) |
| 2235        |   | 446 (M + H) |
| 2236        |  | 484 (M + H) |

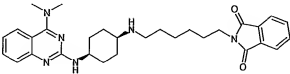
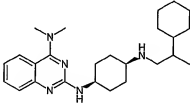
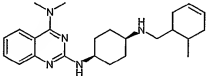
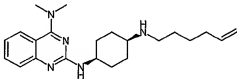
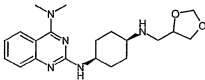


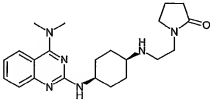
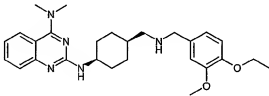
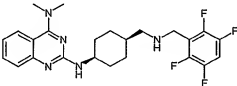
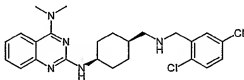
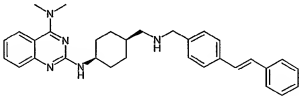
| Example No. | Structure  | APCI-MS     |
|-------------|--|-------------|
| 2237        |   | 420 (M + H) |
| 2238        |   | 568 (M + H) |
| 2239        |   | 428 (M + H) |
| 2240        |   | 396 (M + H) |
| 2241        |  | 420 (M + H) |

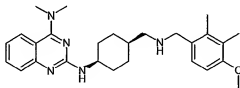
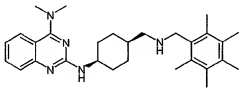
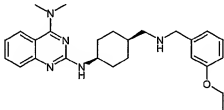
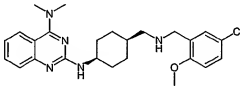
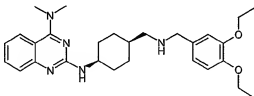
| Example No. | Structure  | APCI-MS     |
|-------------|--|-------------|
| 2242        |   | 468 (M + H) |
| 2243        |   | 432 (M + H) |
| 2244        |   | 468 (M + H) |
| 2245        |   | 458 (M + H) |
| 2246        |  | 423 (M + H) |

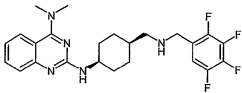
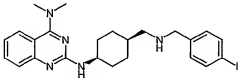
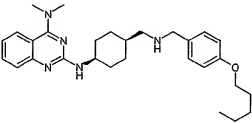
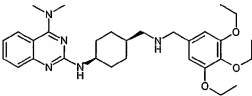
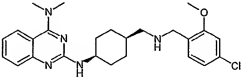
| Example No. | Structure  | APCI-MS     |
|-------------|--|-------------|
| 2247        |   | 420 (M + H) |
| 2248        |   | 404 (M + H) |
| 2249        |   | 448 (M + H) |
| 2250        |   | 446 (M + H) |
| 2251        |  | 540 (M + H) |

| Example No. | Structure  | APCI-MS     |
|-------------|--|-------------|
| 2252        |   | 470 (M + H) |
| 2253        |   | 472 (M + H) |
| 2254        |   | 479 (M + H) |
| 2255        |   | 433 (M + H) |
| 2256        |  | 458 (M + H) |

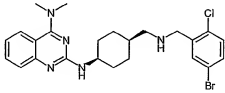
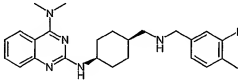
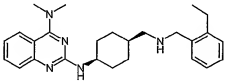
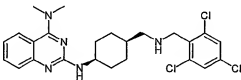
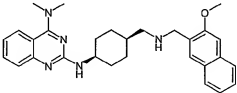
| Example No. | Structure  | APCI-MS     |
|-------------|--|-------------|
| 2257        |   | 515 (M + H) |
| 2258        |   | 410 (M + H) |
| 2259        |   | 394 (M + H) |
| 2260        |   | 368 (M + H) |
| 2261        |  | 372 (M + H) |

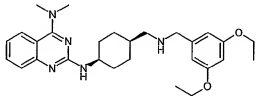
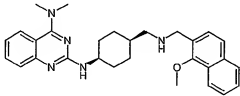
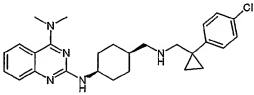
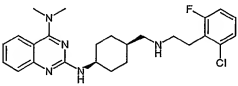
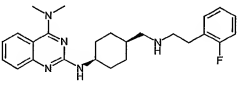
| Example No. | Structure  | APCI-MS     |
|-------------|--|-------------|
| 2262        |   | 397 (M + H) |
| 2263        |   | 464 (M + H) |
| 2264        |   | 462 (M + H) |
| 2265        |   | 458 (M + H) |
| 2266        |  | 492 (M + H) |

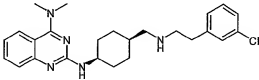
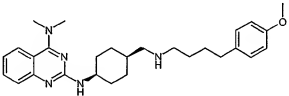
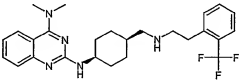
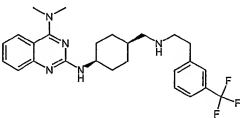
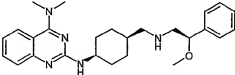
| Example No. | Structure  | APCI-MS     |
|-------------|--|-------------|
| 2267        |   | 448 (M + H) |
| 2268        |   | 460 (M + H) |
| 2269        |   | 434 (M + H) |
| 2270        |   | 454 (M + H) |
| 2271        |  | 478 (M + H) |

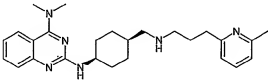
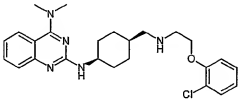
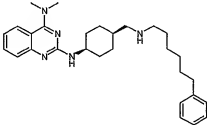
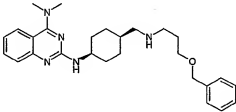
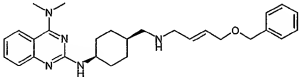
| Example No. | Structure  | APCI-MS     |
|-------------|--|-------------|
| 2272        |   | 462 (M + H) |
| 2273        |   | 516 (M + H) |
| 2274        |   | 476 (M + H) |
| 2275        |   | 522 (M + H) |
| 2276        |  | 454 (M + H) |

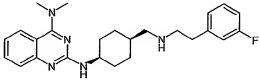
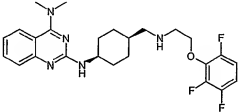
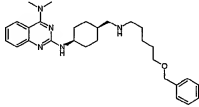
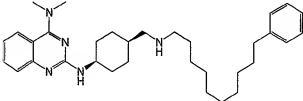
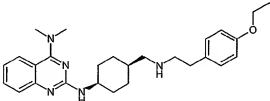


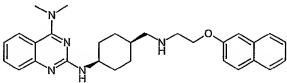
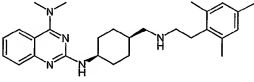
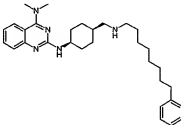
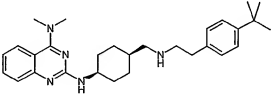
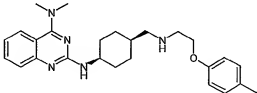
| Example No. | Structure  | APCI-MS     |
|-------------|--|-------------|
| 2277        |   | 502 (M + H) |
| 2278        |   | 530 (M + H) |
| 2279        |   | 418 (M + H) |
| 2280        |   | 492 (M + H) |
| 2281        |  | 470 (M + H) |

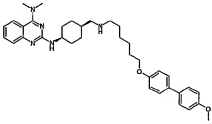
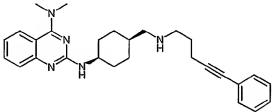
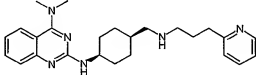
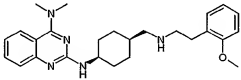
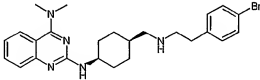
| Example No. | Structure  | APCI-MS     |
|-------------|--|-------------|
| 2282        |   | 478 (M + H) |
| 2283        |   | 470 (M + H) |
| 2284        |   | 464 (M + H) |
| 2285        |   | 456 (M + H) |
| 2286        |  | 422 (M + H) |

| Example No. | Structure  | APCI-MS     |
|-------------|--|-------------|
| 2287        |   | 438 (M + H) |
| 2288        |   | 462 (M + H) |
| 2289        |   | 472 (M + H) |
| 2290        |   | 472 (M + H) |
| 2291        |  | 434 (M + H) |

| Example No. | Structure  | APCI-MS     |
|-------------|--|-------------|
| 2292        |   | 433 (M + H) |
| 2293        |   | 454 (M + H) |
| 2294        |   | 460 (M + H) |
| 2295        |   | 448 (M + H) |
| 2296        |  | 460 (M + H) |

| Example No. | Structure  | APCI-MS     |
|-------------|--|-------------|
| 2297        |   | 422 (M + H) |
| 2298        |   | 474 (M + H) |
| 2299        |   | 476 (M + H) |
| 2300        |   | 516 (M + H) |
| 2301        |  | 448 (M + H) |

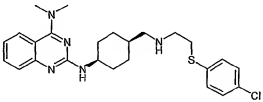
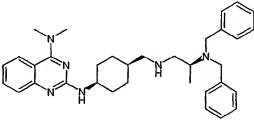
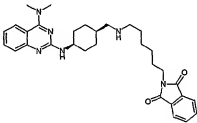
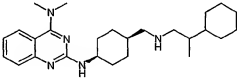
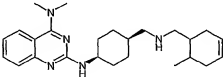
| Example No. | Structure  | APCI-MS     |
|-------------|--|-------------|
| 2302        |   | 470 (M + H) |
| 2303        |   | 446 (M + H) |
| 2304        |   | 488 (M + H) |
| 2305        |   | 460 (M + H) |
| 2306        |  | 434 (M + H) |

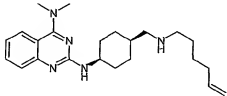
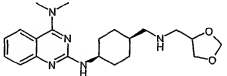
| Example No. | Structure  | APCI-MS     |
|-------------|--|-------------|
| 2307        |   | 582 (M + H) |
| 2308        |   | 442 (M + H) |
| 2309        |   | 419 (M + H) |
| 2310        |   | 434 (M + H) |
| 2311        |  | 482 (M + H) |



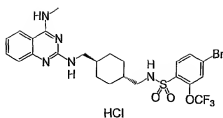




| Example No. | Structure  | APCI-MS     |
|-------------|--|-------------|
| 2322        |   | 470 (M + H) |
| 2323        |   | 537 (M + H) |
| 2324        |   | 529 (M + H) |
| 2325        |   | 424 (M + H) |
| 2326        |  | 408 (M + H) |

| Example No. | Structure  | APCI-MS     |
|-------------|--|-------------|
| 2327        | <br><chem>CN(C)c1nc2ccccc2n1NC3CCCCC3CCNCCCC=C</chem>   | 382 (M + H) |
| 2328        | <br><chem>CN(C)c1nc2ccccc2n1NC3CCCCC3CCNCC4OCCO4</chem> | 386 (M + H) |

## Example 2329



***trans*-4-Bromo-N-[(4-methylamino-quinazolin-2-ylamino)-methyl]-cyclohexylmethyl]-2-trifluoromethoxy-benzenesulfonamide hydrochloride**

**Step A: Synthesis of *trans*-4-[(4-bromo-2-trifluoromethoxy-benzenesulfonylamino)-methyl]-cyclohexanecarboxylic acid.**

To a solution of *trans*-4-aminomethyl-cyclohexanecarboxylic acid (3.14 g, 20 mmol) in THF (20 mL) and 1 M aqueous sodium hydroxide (42 mL) was added a solution of 4-bromo-2-trifluoromethoxy benzenesulfonyl chloride (6.9 g, 20.4 mmol) in THF (20 mL) and the mixture was stirred for 2 hr at ambient temperature. The resulting mixture was concentrated and 1 M aqueous HCl (45 mL) was added. The resulting precipitate was filtered, washed with water and hexanes to give *trans*-4-[(4-bromo-2-trifluoromethoxy-benzenesulfonylamino)-methyl]-cyclohexanecarboxylic acid (7.18 g, 78%) as a white powder.

ESI MS  $m/e$  460/462  $M + H^+$ ;  $^1H$  NMR (500 MHz, DMSO- $d_6$ )  $\delta$  12.00 (brs, 1 H), 7.99 (brs, 1 H), 7.84-7.80 (m, 3 H), 2.72 (d,  $J = 6.3$  Hz, 2 H), 2.10 (m, 1 H), 1.86 (m, 2 H), 1.71 (m, 2 H), 1.31 (m, 1 H), 1.23 (m, 2 H), 0.87 (m, 2 H).

**Step B: Synthesis of *trans*-4-[(4-bromo-2-trifluoromethoxy-benzenesulfonylamino)-methyl]-cyclohexanecarboxylic acid amide.**

A solution of *trans*-4-[(4-bromo-2-trifluoromethoxy-benzenesulfonylamino)-methyl]-cyclohexanecarboxylic acid (7.14 g, 15.5 mmol) and triethylamine (2.35 mL, 16.9 mmol) in THF (25 mL) was cooled to 0 °C. To the mixture was added ethyl chloroformate (1.62 mL, 17 mmol) in THF (5 mL) over 10 min. After stirring at 0 °C for 15 min, aqueous ammonia (27 mL) was added dropwise and the mixture was stirred at ambient temperature for 2 hr. The mixture was concentrated under reduced pressure and the concentrate was treated with water to give a solid. The solid was filtered and washed with water and hexanes to give *trans*-4-[(4-bromo-2-trifluoromethoxy-

806

benzenesulfonylamino)-methyl]-cyclohexanecarboxylic acid amide as a white solid (4.2 g, 59%).

ESI MS  $m/e$  459/461  $M + H^+$ ;  $^1H$  NMR (500 MHz, DMSO- $d_6$ )  $\delta$  7.98 (brs, 1 H), 7.84-7.80 (m, 3 H), 7.13 (s, 1 H), 6.62 (s, 1 H), 2.72 (d,  $J = 6.5$  Hz, 2 H), 1.98 (m, 1 H), 1.70 (m, 4 H), 1.29 (m, 1 H), 1.23 (m, 2 H), 0.83 (m, 2 H).

**Step C: Synthesis of *trans*-*N*-(4-aminomethyl-cyclohexylmethyl)-4-bromo-2-trifluoromethoxy-benzenesulfonamide.**

To a solution of *trans*-4-[(4-bromo-2-trifluoromethoxy-benzenesulfonylamino)-methyl]-cyclohexanecarboxylic acid amide (4.2 g, 9.2 mmol) in THF (40 mL) was added a solution of 1 M  $BH_3$  in THF (32 mL, 32 mmol) over 40 min. The mixture was refluxed for 2 hr. After cooling to 0 °C, the mixture was quenched with water (7 mL). To the resulting mixture were added 4 M HCl in EtOAc (28 mL) and MeOH (28 mL) and the mixture was concentrated. To the residue was added MeOH (28 mL) and the mixture was once again concentrated. The resulting HCl-salt was recrystallized from Et<sub>2</sub>O and subsequently neutralized with 1 M aqueous sodium hydroxide. The aqueous layer was extracted with  $CH_2Cl_2$  (twice), the organic layers combined, dried over sodium sulfate, and concentrated under reduced pressure to give *trans*-*N*-(4-aminomethyl-cyclohexylmethyl)-4-bromo-2-trifluoromethoxy-benzenesulfonamide as a white solid (3.0 g, 74%).

ESI MS  $m/e$  445/447  $M + H^+$ ;  $^1H$  NMR (500 MHz, DMSO- $d_6$ )  $\delta$  7.84-7.79 (m, 3 H), 3.42 (brs, 2 H), 2.72 (d,  $J = 6.8$  Hz, 2 H), 2.33 (d,  $J = 6.5$  Hz, 2 H), 1.73 (m, 4 H), 1.27 (m, 1 H), 1.09 (m, 1 H), 0.80 (m, 4 H).

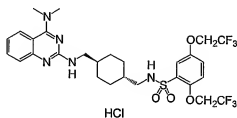
**Step D: Synthesis of *trans*-4-Bromo-*N*-{4-[(4-methylamino-quinazolin-2-ylamino)-methyl]-cyclohexylmethyl}-2-trifluoromethoxy-benzenesulfonamide hydrochloride.**

A mixture of (2-chloro-quinazolin-4-yl)-methylamine obtained in step A of example 50 (58 mg, 0.3 mmol) and *trans*-*N*-(4-aminomethyl-cyclohexylmethyl)-4-bromo-2-trifluoromethoxy-benzenesulfonamide amide (133 mg, 0.3 mmol) in 2-propanol (0.5 mL) was stirred at reflux for 24 hr. The mixture was cooled and the resulting white solid was collected by filtration and washed with 2-propanol to give *trans*-4-Bromo-*N*-{4-[(4-methylamino-quinazolin-2-ylamino)-methyl]-cyclohexylmethyl}-2-trifluoromethoxy-benzenesulfonamide hydrochloride as a white solid (121 mg, 67%).

ESI MS  $m/e$  602/604  $M + H^+$ ;  $^1H$  NMR (500 MHz, DMSO- $d_6$ )  $\delta$  12.61 (brs, 1 H), 9.70

(brs, 1 H), 8.26 (d,  $J = 8.1$  Hz, 1 H), 8.15 (brs, 1 H), 8.02 (t,  $J = 5.7$  Hz, 1 H), 7.84-7.74 (m, 4 H), 7.41 (m, 1 H), 3.32 (m, 2 H), 3.07 (d,  $J = 3.5$  Hz, 3 H), 2.73 (t,  $J = 6.2$  Hz, 2 H), 1.77 (m, 4 H), 1.53 (m, 1 H), 1.32 (m, 1 H), 0.96 (m, 2 H), 0.82 (m, 2 H).

### Example 2330



***trans*-N-{4-[(4-Dimethylamino-quinazolin-2-ylamino)-methyl]-cyclohexylmethyl}-2,5-bis-(2,2,2-trifluoro-ethoxy)-benzenesulfonamide hydrochloride**

#### Step A: Synthesis of *trans*-4-{[2,5-bis-(2,2,2-trifluoro-ethoxy)-benzenesulfonylamino]-methyl}-cyclohexanecarboxylic acid.

To a solution of *trans*-4-aminomethyl-cyclohexanecarboxylic acid (1.5 g, 10 mmol) in THF (10 mL) and 1 M aqueous sodium hydroxide (27 mL) was added a solution of 2,5-bis(2,2,2-trifluoroethoxy) benzenesulfonyl chloride (3.8 g, 10.25 mmol) in THF (10 mL) dropwise and the mixture was stirred at ambient temperature for 2 hr. The resulting mixture was concentrated and 1 M aqueous HCl (22.5 mL) was added. The resulting precipitate was filtered, washed with water and hexanes to give *trans*-4-{[2,5-bis-(2,2,2-trifluoro-ethoxy)-benzenesulfonylamino]-methyl}-cyclohexanecarboxylic acid as a white powder (2.8 g, 57%).

ESI MS  $m/e$  494  $M + H^+$ ;  $^1H$  NMR (500 MHz, DMSO- $d_6$ )  $\delta$  7.36 (m, 3 H), 7.23 (brs, 1 H), 4.88 (m, 4 H), 2.73 (m, 2 H), 2.10 (m, 1 H), 1.87 (m, 2 H), 1.72 (m, 2 H), 1.30 (m, 1 H), 1.23 (m, 2 H), 0.87 (m, 2 H).

#### Step B: Synthesis of *trans*-4-{[2,5-bis-(2,2,2-trifluoro-ethoxy)-benzenesulfonylamino]-methyl}-cyclohexanecarboxylic acid amide.

A solution of *trans*-4-{[2,5-bis-(2,2,2-trifluoro-ethoxy)-benzenesulfonylamino]-methyl}-cyclohexanecarboxylic acid (2.78 g, 5.63 mmol) and triethylamine (1.9 mL,

13.6 mmol) in THF (25 mL) was cooled to 0 °C. To the mixture was added ethyl chloroformate (0.586 mL, 6.2 mmol) in THF (5 mL) over 10 min. After stirring at 0 °C for 15 min, 25% aqueous ammonia (10 mL) was added dropwise. The mixture was stirred at ambient temperature for 2 hr. The resulting mixture was concentrated under reduced pressure and the concentrate was diluted with water to give a solid. The solid was filtered and washed with water and hexanes to give *trans*-4-([2,5-bis-(2,2,2-trifluoro-ethoxy)-benzenesulfonylamino]-methyl)-cyclohexanecarboxylic acid amide as a white solid (2.7 g, 98%).

ESI MS *m/e* 493 *M* + *H*<sup>+</sup>; <sup>1</sup>H NMR (500 MHz, DMSO-*d*<sub>6</sub>) δ 7.36 (m, 3 H), 7.23 (t, *J* = 6.1 Hz, 1 H), 7.13 (s, 1 H), 6.62 (s, 1 H), 4.88 (m, 4 H), 2.74 (t, *J* = 6.4 Hz, 2 H), 1.99 (m, 1 H), 1.75 (m, 4 H), 1.28 (m, 1 H), 1.23 (m, 2 H), 0.83 (m, 2 H).

**Step C: Synthesis of *trans*-*N*-(4-aminomethyl-cyclohexylmethyl)-2,5-bis-(2,2,2-trifluoro-ethoxy)-benzenesulfonamide.**

To a solution of *trans*-4-([2,5-bis-(2,2,2-trifluoro-ethoxy)-benzenesulfonylamino]-methyl)-cyclohexanecarboxylic acid amide (2.7 g, 5.5 mmol) in THF (20 mL) was added a solution of 1 M BH<sub>3</sub> in THF (20 mL, 20 mmol) over 40 min. The mixture was stirred at reflux for 2 hr. After cooling to 0 °C, the mixture was quenched with water (7 mL). To the mixture were added 4 M HCl in EtOAc (28 mL) and MeOH (50 mL) and the mixture was concentrated. To the residue was added MeOH (50 mL) and the mixture was once again concentrated. The resulting HCl-salt was recrystallized from Et<sub>2</sub>O and subsequently neutralized with 1 M aqueous sodium hydroxide. The aqueous layer was extracted with CH<sub>2</sub>Cl<sub>2</sub> (twice), the combined organic layers were dried over sodium sulfate, and concentrated under reduced pressure to give *trans*-*N*-(4-aminomethyl-cyclohexylmethyl)-2,5-bis-(2,2,2-trifluoro-ethoxy)-benzenesulfonamide as a white solid (1.5 g, 57%).

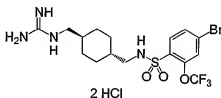
ESI MS *m/e* 479 *M* + *H*<sup>+</sup>; <sup>1</sup>H NMR (500 MHz, DMSO-*d*<sub>6</sub>) δ 7.36-7.32 (m, 3 H), 6.62 (brs, 1 H), 4.88-4.78 (m, 4 H), 3.42 (b, 2 H), 2.73 (d, *J* = 6.6 Hz, 2 H), 2.34 (d, *J* = 6.3 Hz, 2 H), 1.73 (m, 4 H), 1.27 (m, 1 H), 1.10 (m, 1 H), 0.77 (m, 4 H).

**Step D: Synthesis of *trans*-*N*-[4-[(4-Dimethylamino-quinazolin-2-ylamino)-methyl]-cyclohexylmethyl]-2,5-bis-(2,2,2-trifluoro-ethoxy)-benzenesulfonamide hydrochloride.**

A mixture of (2-chloro-quinazoline-4-yl)-dimethyl-amine obtained in step B of example 1 (41.4 mg, 0.2 mmol) and *trans*-*N*-(4-aminomethyl-cyclohexylmethyl)-2,5-bis-(2,2,2-trifluoro-ethoxy)-benzenesulfonamide (95.6 mg, 0.2 mmol) in 2-propanol was stirred at reflux for 24 hr. The reaction mixture was concentrated and the residue was purified by column chromatography (silica gel) to give the product as a white foam. The product was dissolved in  $\text{CH}_2\text{Cl}_2$  and treated with 1 M HCl in  $\text{Et}_2\text{O}$ . The mixture was concentrated to give *trans*-*N*-{4-[(4-Dimethylamino-quinazolin-2-ylamino)-methyl]-cyclohexylmethyl}-2,5-bis-(2,2,2-trifluoro-ethoxy)-benzenesulfonamide hydrochloride as a white foam (101 mg, 78%).

ESI MS  $m/e$  650  $M + H^+$ ;  $^1\text{H}$  NMR (500 MHz,  $\text{DMSO}-d_6$ )  $\delta$  8.16 (d,  $J = 8.2$  Hz, 1 H), 8.00 (brs, 1 H), 7.78 (t,  $J = 7.9$ , 1 H), 7.44 (brs, 1 H), 7.34 (m, 4 H), 7.24 (t,  $J = 5.9$  Hz, 1 H), 4.88 (m, 4 H), 3.32 (s, 6 H), 3.29 (m, 2 H), 2.75 (t,  $J = 6.2$  Hz, 2 H), 1.74 (m, 4 H), 1.52 (m, 1 H), 1.32 (m, 1 H), 0.94 (m, 2 H), 0.83 (m, 2 H).

#### Example 2331



***trans*-4-Bromo-*N*-(4-guanidinomethyl-cyclohexylmethyl)-2-trifluoromethoxy-benzenesulfonamide dihydrochloride**

**Step A: Synthesis of *trans*-{[4-[(4-bromo-2-trifluoromethoxy-benzenesulfonylamino)-methyl]-cyclohexylmethyl]-amino}-*tert*-butoxycarbonylamino-methyl]-carbamic acid *tert*-butyl ester.**

To a solution of *trans*-*N*-(4-aminomethyl-cyclohexylmethyl)-4-bromo-2-trifluoromethoxy-benzenesulfonamide obtained in step C of example 2329 (45 mg, 0.1 mmol) and triethylamine (14  $\mu\text{L}$ , 0.1 mmol) in  $\text{CH}_2\text{Cl}_2$  (5 mL) was added (*tert*-butoxycarbonylamino-trifluoromethanesulfonylimino-methyl)-carbamic acid *tert*-butyl ester (39.1 mg, 0.1 mmol). The reaction mixture was stirred at ambient temperature for 2 hr and concentrated. The residue was purified by column chromatography (silica gel,



$\text{CH}_2\text{Cl}_2$  to 10% MeOH in  $\text{CH}_2\text{Cl}_2$ ) to give *trans*-[({4-[4-bromo-2-trifluoromethoxy-benzenesulfonylamino)-methyl]-cyclohexylmethyl}-amino)-*tert*-butoxycarbonylamino-methyl]-carbamic acid *tert*-butyl ester as a white solid (63 mg, 92%).

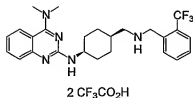
ESI MS  $m/e$  687/689  $\text{M} + \text{H}^+$ ;  $^1\text{H}$  NMR (400 MHz,  $\text{DMSO}-d_6$ )  $\delta$  11.45 (s, 1 H), 8.22 (t,  $J = 5.6$  Hz, 1 H), 7.97 (t,  $J = 5.6$  Hz, 1 H), 7.99-7.79 (m, 3 H), 3.13 (t,  $J = 6.4$  Hz, 2 H), 2.72 (t,  $J = 6$  Hz, 2 H), 1.70 (m, 4 H), 1.46 (s, 9 H), 1.38 (s, 9 H), 1.31 (m, 2 H), 0.83 (m, 4 H).

**Step B: Synthesis of *trans*-4-bromo-*N*-(4-guanidinomethyl-cyclohexylmethyl)-2-trifluoromethoxy-benzenesulfonamide dihydrochloride.**

A solution of *trans*-[({4-[4-bromo-2-trifluoromethoxy-benzenesulfonylamino)-methyl]-cyclohexylmethyl}-amino)-*tert*-butoxycarbonylamino-methyl]-carbamic acid *tert*-butyl ester (53 mg, 0.077 mmol) in 50% TFA in  $\text{CH}_2\text{Cl}_2$  (2 mL) was stirred at ambient temperature for 3 hr and the reaction mixture was concentrated. To the residue was added a solution of 1 M HCl in  $\text{Et}_2\text{O}$  (0.5 mL) and the mixture was concentrated to give *trans*-4-Bromo-*N*-(4-guanidinomethyl-cyclohexylmethyl)-2-trifluoromethoxy-benzenesulfonamide dihydrochloride as a white solid (29 mg, 68%).

ESI MS  $m/e$  487/489  $\text{M} + \text{H}^+$ ;  $^1\text{H}$  NMR (500 MHz,  $\text{DMSO}-d_6$ )  $\delta$  8.01 (t,  $J = 5.5$  Hz, 1 H), 7.84 (m, 3 H), 7.68 (m, 1 H), 7.30 (m, 2 H), 6.85 (m, 2 H), 2.94 (t,  $J = 6.1$  Hz, 2 H), 2.74 (t,  $J = 6.1$  Hz, 2 H), 1.71 (m, 2 H), 1.31 (m, 4 H), 0.86 (m, 4 H).

**Example 2332**



*cis*- $N',N'$ -Dimethyl- $N''$ -[4-[(2-trifluoromethyl-benzylamino)-methyl]-cyclohexyl]-quinazoline-2,4-diamine ditrifluoro-acetic acid

**Step A: Synthesis of *cis*-4-*tert*-butoxycarbonylamino-cyclohexanecarboxylic acid.**

To a solution of *cis*-4-amino-cyclohexanecarboxylic acid (50 g, 350 mmol) in THF

(200 mL) and 1 M aqueous sodium hydroxide (380 mL, 380 mmol) was added ( $\text{Boc}_2\text{O}$  (83.5 g, 360 mmol). The reaction mixture was stirred at ambient temperature for 2 hr and concentrated. The residue was cooled to 0 °C followed by acidification with 1 M HCl (pH = 3). The resulting white solid was filtered, washed with water and hexanes to give *cis*-4-*tert*-butoxycarbonylamino-cyclohexanecarboxylic acid (71 g, 83%) as a white solid. ESI MS  $m/e$  244  $\text{M} + \text{H}^+$ ;  $^1\text{H}$  NMR (400 MHz,  $\text{DMSO-d}_6$ )  $\delta$  12.00 (brs, 1 H), 6.74 (d,  $J$  = 4.25, 1 H), 3.30 (brs, 1 H), 2.35 (m, 1 H), 1.87 (m, 2 H), 1.55-1.37 (m, 15 H).

**Step B: Synthesis of *cis*-(4-carbamoyl-cyclohexyl)-carbamic acid *tert*-butyl ester.**

To a solution cooled at 0 °C of *cis*-4-*tert*-butoxycarbonylamino-cyclohexanecarboxylic acid (68.0 g, 280 mmol) and triethylamine (31.1 g, 307 mmol) in THF (300 mL) was added ethyl chloroformate (29.3 mL, 308 mmol) dropwise. After stirring at 0 °C for 30 min, 25% aqueous ammonia (168 mL) was added dropwise. The reaction mixture was stirred at ambient temperature for 2 hr and concentrated. The residue was extracted with EtOAc (three times). The combined organic layer was washed with saturated aqueous  $\text{NaHCO}_3$ , 1 M HCl, brine, and water, dried over  $\text{Na}_2\text{SO}_4$ , filtered, and concentrated to give *cis*-(4-carbamoyl-cyclohexyl)-carbamic acid *tert*-butyl ester (62.0 g, 88%) as a white solid.

ESI MS  $m/e$  243  $\text{M} + \text{H}^+$ ;  $^1\text{H}$  NMR (400 MHz,  $\text{DMSO-d}_6$ )  $\delta$  7.10 (brs, 1 H), 6.69 (b, 2 H), 3.41 (brs, 1 H), 2.14 (m, 1 H), 1.79 (m, 2 H), 1.59 (m, 2 H), 1.45-1.37 (m, 13 H).

**Step C: Synthesis of *cis*-4-amino-cyclohexanecarboxylic acid amide hydrochloride.**

To a solution of *cis*-(4-carbamoyl-cyclohexyl)-carbamic acid *tert*-butyl ester (62 g, 256 mmol) in  $\text{CH}_2\text{Cl}_2$  (250 mL) was added TFA (250 mL) and the mixture was stirred at ambient temperature for 1 hr. The mixture was concentrated and 2 M HCl in  $\text{Et}_2\text{O}$  (150 mL) was added to give a white precipitate. The mixture was concentrated to give *cis*-4-amino-cyclohexanecarboxylic acid amide hydrochloride (45 g, 98%) as a white solid.

ESI MS  $m/e$  143  $\text{M} + \text{H}^+$ ;  $^1\text{H}$  NMR (400 MHz,  $\text{DMSO-d}_6$ )  $\delta$  8.08 (m, 3 H), 7.28 (s, 1 H), 6.78 (s, 1 H), 3.10 (m, 1 H), 2.24 (m, 1 H), 1.90 (m, 2 H), 1.66 (m, 4 H), 1.50 (m, 2 H).

**Step D: Synthesis of *cis*-4-(4-dimethylamino-quinazolin-2-ylamino)-cyclohexanecarboxylic acid amide.**

A solution of (2-chloro-quinazolin-4-yl)-dimethyl-amine obtained in step B of

example 1 (31.05 g, 150 mmol) and *cis*-4-amino-cyclohexanecarboxylic acid amide hydrochloride (26.7 g, 150 mmol) in pyridine (150 mL) was stirred at reflux for overnight. The reaction mixture was concentrated and residue was dissolve in  $\text{CH}_2\text{Cl}_2$ . The organic layer was washed with saturated aqueous  $\text{NaHCO}_3$  and the aqueous layer was extracted with  $\text{CH}_2\text{Cl}_2$ . The organic layer was dried over  $\text{Na}_2\text{SO}_4$ , filtered and concentrated. The residue was purified by column chromatography (silica gel, 2% to 10% 2 M  $\text{NH}_3/\text{MeOH}$  in  $\text{CH}_2\text{Cl}_2$ ) to give a slightly brown solid and the solid was recrystallized from  $\text{CH}_2\text{Cl}_2$  to give *cis*-4-(4-dimethylamino-quinazolin-2-ylamino)-cyclohexanecarboxylic acid amide (20.6 g, 44%) as yellow crystals.

ESI MS  $m/e$  314  $\text{M} + \text{H}^+$ ;  $^1\text{H}$  NMR (400 MHz,  $\text{DMSO}-d_6$ )  $\delta$  8.19 (brs, 1 H), 8.15 (d,  $J = 8.4$  Hz, 1 H), 7.77 (t,  $J = 8.0$  Hz, 1 H), 7.42 (d,  $J = 7.2$  Hz, 1 H), 7.35 (t,  $J = 8.4$  Hz, 1 H), 7.21 (s, 1 H), 6.74 (s, 1 H), 4.12 (m, 1 H), 3.46 (m, 6 H), 2.24 (m, 1 H), 1.79-1.61 (m, 8 H).

**Step E: Synthesis of *cis*- $N^2$ -(4-aminomethyl-cyclohexyl)- $N^4$ , $N^4$ -dimethyl-quinazoline-2,4-diamine.**

To a solution of *cis*-4-(4-dimethylamino-quinazolin-2-ylamino)-cyclohexanecarboxylic acid amide (18.78 g, 60 mmol) in THF (200 mL) was added a solution of 1 M  $\text{BH}_3$  in THF (300 mL, 300 mmol). The mixture was stirred at reflux for 2 hr. After cooling the reaction mixture to 0  $^\circ\text{C}$ , 4 M  $\text{HCl}$  in  $\text{EtOAc}$  (100 mL) and  $\text{MeOH}$  (200 mL) were added. The mixture was concentrated. The mixture was treated with 1 M aqueous sodium hydroxide and the aqueous layer was extracted with  $\text{CH}_2\text{Cl}_2$ . The organic layer was dried over sodium sulfate, concentrated, and purified by column chromatography (silica gel, 10% 2 M  $\text{NH}_3/\text{MeOH}$  in  $\text{CH}_2\text{Cl}_2$ ) to give *cis*- $N^2$ -(4-aminomethyl-cyclohexyl)- $N^4$ , $N^4$ -dimethyl-quinazoline-2,4-diamine as a white solid (10.6 g, 59%).

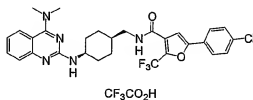
ESI MS  $m/e$  300  $\text{M} + \text{H}^+$ ;  $^1\text{H}$  NMR (400 MHz,  $\text{DMSO}-d_6$ )  $\delta$  7.84 (d,  $J = 8.4$  Hz, 1 H), 7.46 (t,  $J = 6.8$  Hz, 1 H), 7.26 (d,  $J = 8.4$  Hz, 1 H), 6.99 (t,  $J = 6.8$  Hz, 1 H), 6.28 (brs, 1 H), 4.02 (m, 1 H), 3.19 (m, 6 H), 2.47 (d,  $J = 6.8$  Hz, 2 H), 2.73 (m 2 H), 1.68-1.33 (m, 9 H).

**Step F: Synthesis of *cis*- $N^4$ , $N^4$ -dimethyl- $N^2$ -{4-[(2-trifluoromethyl-benzylamino)-methyl]-cyclohexyl}-quinazoline-2,4-diamine ditrifluoro-acetic acid.**

A solution of *cis*-*N*<sup>2</sup>-(4-aminomethyl-cyclohexyl)-*N*<sup>4</sup>,*N*<sup>4</sup>-dimethyl-quinazoline-2,4-diamine (33 mg, 0.11 mmol) and 2-trifluoromethyl benzaldehyde (17.41 mg, 0.1 mmol) in MeOH (1 mL) was stirred at ambient temperature for 3 hr. To the mixture was added NaBH(OAc)<sub>3</sub> (85 mg, 0.4 mmol) and the mixture was stirred at ambient temperature for overnight. This resulting mixture was quenched with 50% DMSO in water (2 mL) and the solution was purified by preparative HPLC. The pure fractions were combined and lyophilized to give *cis*-*N*<sup>4</sup>,*N*<sup>4</sup>-dimethyl-*N*<sup>2</sup>-{4-[(2-trifluoromethyl-benzylamino)-methyl]-cyclohexyl}-quinazoline-2,4-diamine ditrifluoro-acetic acid (41.4 mg, 60%) as a white solid.

ESI MS *m/e* 458 M + H<sup>+</sup>; <sup>1</sup>H NMR (400 MHz, DMSO-*d*<sub>6</sub>) δ 13.12 (brs, 1 H), 8.94 (b, 2 H), 8.65 (d, *J* = 6.8 Hz, 1 H), 8.16 (d, *J* = 8.8 Hz, 1 H), 7.77-7.66 (m, 5 H), 7.41 (d, *J* = 8.4 Hz, 1 H), 7.35 (t, *J* = 8 Hz, 1 H), 4.22 (s, 2 H), 4.17 (m, 1 H), 3.46 (b, 6 H), 2.94 (m, 2 H), 1.87-1.44 (m, 9 H).

#### Example 2333



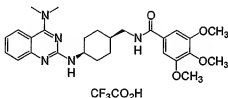
*cis*-5-(4-Chloro-phenyl)-2-trifluoromethyl-furan-3-carboxylic acid [4-(4-dimethylamino-quinazolin-2-ylamino)-cyclohexylmethyl]-amide trifluoro-acetic acid

**Step A: Synthesis of *cis*-5-(4-chloro-phenyl)-2-trifluoromethyl-furan-3-carboxylic acid [4-(4-dimethylamino-quinazolin-2-ylamino)-cyclohexylmethyl]-amide trifluoro-acetic acid.**

A solution of *cis*-*N*<sup>2</sup>-(4-aminomethyl-cyclohexyl)-*N*<sup>4</sup>,*N*<sup>4</sup>-dimethyl-quinazoline-2,4-diamine obtained in step E of example 2332 (30 mg, 0.1 mmol), 5-(4-chloro-phenyl)-2-trifluoromethyl-furan-3-acid chloride (37 mg, 0.12 mmol), and pyridine (12 μL, 0.15 mmol) in DMF (0.5 mL) was stirred at ambient temperature for overnight. The resulting mixture was diluted with DMSO (0.8 mL) and the mixture was purified by preparative

HPLC. The pure fractions were combined and lyophilized to give *cis*-5-(4-chloro-phenyl)-2-trifluoromethyl-furan-3-carboxylic acid [4-(4-dimethylamino-quinazolin-2-ylamino)-cyclohexylmethyl]-amide trifluoro-acetic acid (17.5 mg, 26%) as a white solid. ESI MS  $m/e$  572  $M + H^+$ ;  $^1H$  NMR (400 MHz, DMSO- $d_6$ )  $\delta$  12.30 (brs, 1 H), 8.65 (t,  $J = 6.8$  Hz, 1 H), 8.19 (brs, 1 H), 8.14 (d,  $J = 8.0$  Hz, 1 H), 7.83-7.30 (m, 8 H), 4.1 (m, 1 H), 3.46 (b, 6 H), 3.09 (m, 2 H), 1.77-1.38 (m, 9 H).

### Example 2334



***cis*-N-[4-(4-Dimethylamino-quinazolin-2-ylamino)-cyclohexylmethyl]-3,4,5-trimethoxy-benzamide trifluoro-acetic acid**

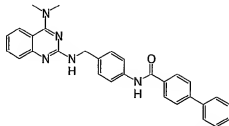
#### Step A: Synthesis of *cis*-N-[4-(4-dimethylamino-quinazolin-2-ylamino)-cyclohexylmethyl]-3,4,5-trimethoxy-benzamide trifluoro-acetic acid.

To HOBT-6-carboxaamidomethyl polystyrene 200-400 mesh (77 mg, 0.1 mmol) were added a solution of 0.3 M PyBroP in DMF (1 mL, 0.3 mmol), 3,4,5-trimethoxybenzoic acid (63 mg, 0.3 mmol), and diisopropylethylamine (85  $\mu$ L, 0.5 mmol). The mixture was stirred at ambient temperature for 5 hr. The resin was washed with DMF (3 times),  $CH_2Cl_2$  (3 times), MeOH (3 times),  $CH_2Cl_2$  (2 times), and DMF (2 times). To the resin was added *cis*-N<sup>2</sup>-(4-aminomethyl-cyclohexyl)-N<sup>4</sup>,N<sup>4</sup>-dimethyl-quinazoline-2,4-diamine obtained in step E of example 2332 (28 mg, 0.09 mmol) in DMF (0.5 mL) and the mixture was stirred at ambient temperature for overnight. The resin was filtered and washed with 0.5 mL DMSO (2 times). The combined filtrates were purified by preparative HPLC. The pure fractions were combined and lyophilized to give *cis* N-[4-(4-dimethylamino-quinazolin-2-ylamino)-cyclohexylmethyl]-3,4,5-trimethoxy-benzamide trifluoro-acetic acid (7.4 mg, 12%) as a white solid.

ESI MS  $m/e$  494  $M + H^+$ ;  $^1H$  NMR (400 MHz, DMSO- $d_6$ )  $\delta$  12.25 (brs, 1 H), 8.45 (t,  $J = 5.6$  Hz, 1 H), 8.17 (brs, 1 H), 8.14 (d,  $J = 8.0$  Hz, 1 H), 7.76 (t,  $J = 8.4$  Hz, 1 H), 7.42 (d,  $J$

= 7.2 Hz, 1 H), 7.34 (t,  $J$  = 7.6 Hz, 1 H), 7.15 (s, 2 H), 4.13 (m, 1 H), 3.44 (s, 3 H), 3.39 (s, 3 H), 3.20 (m, 2 H), 1.77-1.37 (m, 9 H).

### Example 2335



### Biphenyl-4-carboxylic acid {4-[(4-dimethylamino-quinazolin-2-ylamino)-methyl]-phenyl}-amide

#### Step A: Synthesis of (4-amino-benzyl)-carbamic acid *tert*-butyl ester.

A solution of 4-aminomethyl-phenylamine (12.2 g, 100 mmol) and (Boc)<sub>2</sub>O (21.8 g, 100 mmol) in CH<sub>2</sub>Cl<sub>2</sub> (100 mL) was stirred at ambient temperature for overnight. The mixture was concentrated and the residue was purified by column chromatography (silica gel, CH<sub>2</sub>Cl<sub>2</sub> to 10% MeOH in CH<sub>2</sub>Cl<sub>2</sub>) to give (4-amino-benzyl)-carbamic acid *tert*-butyl ester (11.6 g, 52%) as a slightly yellow solid.

ESI MS  $m/e$  223 M + H<sup>+</sup>; <sup>1</sup>H NMR (400 MHz, DMSO-*d*<sub>6</sub>)  $\delta$  7.27 (t,  $J$  = 6.0 Hz, 1 H), 6.86 (d,  $J$  = 8.0 Hz, 2 H), 6.47 (d,  $J$  = 6.4 Hz, 2 H), 4.89 (s, 2 H), 3.91 (d,  $J$  = 6.0 Hz, 2 H), 1.39 (s, 9 H).

#### Step B: Synthesis of biphenyl-4-carboxylic acid (4-aminomethyl-phenyl)-amide hydrochloride.

To a solution of (4-amino-benzyl)-carbamic acid *tert*-butyl ester (1.11 g, 5 mmol), biphenyl carboxylic acid (0.99 g, 5 mmol), EDC (1.2 g, 6.25 mmol), and HOAt (0.82 g, 6 mmol) in CH<sub>2</sub>Cl<sub>2</sub> (10 mL) was added triethylamine (pH = 10) and the mixture was stirred at ambient temperature for overnight. The organic layer was washed with saturated aqueous NaHCO<sub>3</sub>, 1 M aqueous HCl, water, dried over Na<sub>2</sub>SO<sub>4</sub>, filtered, and concentrated. The residue was dissolved in 50% TFA in CH<sub>2</sub>Cl<sub>2</sub> (10 mL) and the mixture was stirred at ambient temperature. After 30 minutes, the mixture was concentrated and diluted with 1 M HCl in Et<sub>2</sub>O (5 mL). The mixture was concentrated to give biphenyl-4-carboxylic acid (4-aminomethyl-phenyl)-amide hydrochloride (828 mg, 49%).

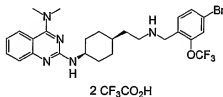
ESI MS  $m/e$  303  $M + H^+$ ;  $^1H$  NMR (400 MHz, DMSO- $d_6$ )  $\delta$  10.40 (s, 1 H), 8.34 (b, 3 H), 8.07 (d,  $J = 8.0$  Hz, 2 H), 7.83-7.73 (m, 6 H), 7.51-7.38 (m, 5 H), 4.0 (q,  $J = 5.6$  Hz, 2 H).

**Step C: Synthesis of biphenyl-4-carboxylic acid {4-[(4-dimethylamino-quinazolin-2-ylamino)-methyl]-phenyl}-amide.**

A mixture of (2-chloro-quinazolin-4-yl)-dimethyl-amine obtained in step B of example 1 (42 mg, 0.2 mmol) and biphenyl-4-carboxylic acid (4-aminomethyl-phenyl)-amide hydrochloride (49 mg, 0.14 mmol) in 2-propanol (1 mL) and triethylamine (200  $\mu$ L) was stirred at reflux for 2 days. The resulting mixture was concentrated and purified by column chromatography (silica gel,  $CH_2Cl_2$  to 10% 2 M  $NH_3/MeOH$  in  $CH_2Cl_2$ ) to give biphenyl-4-carboxylic acid {4-[(4-dimethylamino-quinazolin-2-ylamino)-methyl]-phenyl}-amide (10 mg, 15%) as a white solid.

ESI MS  $m/e$  474  $M + H^+$ ;  $^1H$  NMR (400 MHz, DMSO- $d_6$ )  $\delta$  10.19 (s, 1 H), 8.02 (d,  $J = 7.2$  Hz, 2 H), 7.86 (d,  $J = 8.4$  Hz, 1 H), 7.80 (d,  $J = 8.4$  Hz, 2 H), 7.73 (d,  $J = 7.2$  Hz, 2 H), 7.68 (d,  $J = 7.6$  Hz, 2 H), 7.50-7.15 (m, 8 H), 7.01 (t,  $J = 8.4$  Hz, 1 H), 4.51 (d,  $J = 6.4$  Hz, 2 H), 3.30 (s, 3 H), 3.2 (s, 3 H).

**Example 2336**



*cis*- $N^2$ -[4-[2-(4-Bromo-2-trifluoromethoxy-benzylamino)-ethyl]-cyclohexyl]- $N^4,N^4$ -dimethyl-quinazoline-2,4-diamine ditrifluoro-acetic acid

**Step A: Synthesis of *cis*-[4-(2-benzoyloxycarbonylamino-ethyl)-cyclohexyl]-carbamic acid *tert*-butyl ester.**

To a solution of *cis*-[4-(2-amino-ethyl)-cyclohexyl]-carbamic acid *tert*-butyl ester (4.84 g, 20 mmol) in  $CH_2Cl_2$  (50 mL) and triethylamine (3.06 mL, 22 mmol) was added benzyl chloroformate (3.13 mL, 22 mmol) and the mixture was stirred for 4 hr. The resulting mixture was washed with water, 1 M aqueous HCl, dried over  $Na_2SO_4$ , filtered and concentrated. The residue was purified by column chromatography (silica gel,

$\text{CH}_2\text{Cl}_2$  to 10% MeOH in  $\text{CH}_2\text{Cl}_2$ ) to give *cis*-[4-(2-benzyloxycarbonylamino-ethyl)-cyclohexyl]-carbamic acid *tert*-butyl ester (5.46 g, 73%) as a colorless oil.

ESI MS  $m/e$  377  $M + H^+$ ;  $^1\text{H}$  NMR (400 MHz,  $\text{DMSO}-d_6$ )  $\delta$  7.36-7.24 (m, 5 H), 7.19 (t,  $J = 5.6$  Hz, 1 H), 6.76 (d,  $J = 6.8$  Hz, 1 H), 4.91 (s, 2 H), 3.40 (m, 1 H), 2.99 (m, 2 H), 1.44-1.33 (m, 20H).

**Step B: Synthesis of *cis*-[2-(4-amino-cyclohexyl)-ethyl]-carbamic acid benzyl ester.**

A solution of *cis*-[4-(2-benzyloxycarbonylamino-ethyl)-cyclohexyl]-carbamic acid *tert*-butyl ester (5.26 g, 14 mmol) in 50% TFA in  $\text{CH}_2\text{Cl}_2$  (60 mL) was stirred at ambient temperature for 1 hr. The mixture was concentrated and the residue was diluted with saturated aqueous  $\text{NaHCO}_3$ . The aqueous layer was extracted with  $\text{CH}_2\text{Cl}_2$  (therr times). The organic layer was dried over  $\text{Na}_2\text{SO}_4$  and concentrated to give *cis*-[2-(4-amino-cyclohexyl)-ethyl]-carbamic acid benzyl ester (3.5 g, 91%) as a colorless oil.

ESI MS  $m/e$  277  $M + H^+$ ;  $^1\text{H}$  NMR (400 MHz,  $\text{DMSO}-d_6$ )  $\delta$  7.72 (b, 2 H), 7.34-7.27 (m, 5 H), 7.21 (t,  $J = 5.2$  Hz, 1 H), 4.97 (s, 2 H), 3.14 (m, 1 H), 2.99 (q,  $J = 6.4$  Hz, 2 H), 1.58-1.34 (m, 11 H).

**Step C: Synthesis of *cis*-[2-[4-(4-dimethylamino-quinazolin-2-ylamino)-cyclohexyl]-ethyl]-carbamic acid benzyl ester.**

A mixture of (2-chloro-quinazolin-4-yl)-dimethyl-amine obtained in step B of example 1 (2.45 g, 10.2 mmol) and *cis*-[2-(4-amino-cyclohexyl)-ethyl]-carbamic acid benzyl ester (3.3 g, 10.2 mmol) and triethylamine (1.65 mL, 10.2 mmol) in 2-propanol (15 mL) was heated at 170 °C for 45 min using a Smith Microwave Synthesizer. The mixture was concentrated and the residue was purified by column chromatography (silica gel,  $\text{CH}_2\text{Cl}_2$  to 10% 2 M  $\text{NH}_3/\text{MeOH}$  in  $\text{CH}_2\text{Cl}_2$ ) to give *cis*-[2-[4-(4-dimethylamino-quinazolin-2-ylamino)-cyclohexyl]-ethyl]-carbamic acid benzyl ester (4.48g, 85%) as a yellow oil.

ESI MS  $m/e$  448  $M + H^+$ ;  $^1\text{H}$  NMR (400 MHz,  $\text{DMSO}-d_6$ )  $\delta$  8.07-7.20 (m, 11 H), 4.98 (s, 2 H), 4.08 (m, 1 H), 3.39 (b, 6 H), 3.04 (m, 2 H), 1.7-1.3 (m, 11 H).

**Step D: Synthesis of *cis*- $N^2$ -[4-(2-amino-ethyl)-cyclohexyl]- $N^2$ , $N^2$ -dimethyl-quinazoline-2,4-diamine.**

To a solution of *cis*-[2-[4-(4-dimethylamino-quinazolin-2-ylamino)-cyclohexyl]-



ethyl}-carbamic acid benzyl ester (4.47 g, 10 mmol) in EtOH (20 mL) was added 1,4-cyclohexadiene (20 mL) and 200 mg of 10% Pd/C. The reaction mixture was stirred at ambient temperature for 18 hr, filtered through pad of celite, and concentrated. The residue was purified by column chromatography (silica gel, 5% to 15% 2 M NH<sub>3</sub>/MeOH in CH<sub>2</sub>Cl<sub>2</sub>) to give *cis*-N<sup>2</sup>-[4-(2-amino-ethyl)-cyclohexyl]-N<sup>4</sup>,N<sup>4</sup>-dimethyl-quinazoline-2,4-diamine (2.41 g, 77%) as a yellow oil.

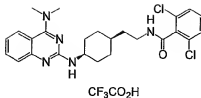
ESI MS *m/e* 314 M + H<sup>+</sup>; <sup>1</sup>H NMR (400 MHz, DMSO-d<sub>6</sub>) δ 7.82 (d, *J* = 8.0 Hz, 1 H), 7.44 (t, *J* = 6.8 Hz, 1 H), 7.27 (d, *J* = 8.0 Hz, 1 H), 6.97 (t, *J* = 6.8 Hz, 1 H), 6.31 (brs, 1 H), 3.97 (m, 1 H), 3.37 (b, 2 H), 3.17 (s, 3), 3.14 (s, 3 H), 2.62 (t, *J* = 7.6 Hz, 2 H), 1.68-1.31 (m, 11 H).

**Step E: Synthesis of *cis*-N<sup>2</sup>-{4-[2-(4-bromo-2-trifluoromethoxy-benzylamino)-ethyl]-cyclohexyl}-N<sup>4</sup>,N<sup>4</sup>-dimethyl-quinazoline-2,4-diamine ditrifluoro-acetic acid.**

A solution of *cis*-N<sup>2</sup>-[4-(2-amino-ethyl)-cyclohexyl]-N<sup>4</sup>,N<sup>4</sup>-dimethyl-quinazoline-2,4-diamine (31.4 mg, 0.1 mmol) and 4-bromo-2-trifluoromethoxy benzaldehyde (26.9 mg, 0.1 mmol) in MeOH (1 mL) was stirred at ambient temperature. After 3 hr, NaBH(OAc)<sub>3</sub> (85 mg, 0.4 mmol) was added and the resulting mixture was stirred at ambient temperature for overnight. The reaction mixture was quenched with 50% DMSO in water (2 mL). The mixture was concentrated and purified by preparative HPLC. The pure fractions were combined and lyophilized to give *cis*-N<sup>2</sup>-{4-[2-(4-bromo-2-trifluoromethoxy-benzylamino)-ethyl]-cyclohexyl}-N<sup>4</sup>,N<sup>4</sup>-dimethyl-quinazoline-2,4-diamine ditrifluoro-acetic acid (32.2 mg, 41%) as a white solid.

ESI MS *m/e* 566/568 M + H<sup>+</sup>; <sup>1</sup>H NMR (400 MHz, DMSO-d<sub>6</sub>) δ 12.76 (brs, 1 H), 8.81 (b, 2 H), 8.43 (m, 1 H), 8.09 (d, *J* = 8.4 Hz, 1 H), 7.71-7.56 (m, 4 H), 7.35 (d, *J* = 8.0 Hz, 1 H), 7.29 (t, *J* = 8.0 Hz, 1 H), 4.15 (m, 3 H), 3.39 (m, 6 H), 2.97 (m, 2 H), 1.67-1.30 (m, 11 H).

## Example 2337



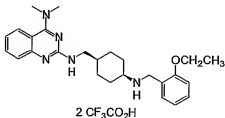
*cis*-2,6-Dichloro-*N*-{2-[4-(4-dimethylamino-quinazolin-2-ylamino)-cyclohexyl]-ethyl}-benzamide trifluoro-acetic acid

**Step A: Synthesis of *cis*-2,6-dichloro-*N*-{2-[4-(4-dimethylamino-quinazolin-2-ylamino)-cyclohexyl]-ethyl}-benzamide trifluoro-acetic acid.**

To a solution of *cis*-*N*<sup>2</sup>-[4-(2-amino-ethyl)-cyclohexyl]-*N*<sup>4</sup>,*N*<sup>4</sup>-dimethyl-quinazoline-2,4-diamine (31.4 mg, 0.1 mmol) and 2,6-dichlorobenzoyl chloride (20.7 mg, 0.1 mmol) in DMF (0.5 mL) was added triethylamine (20 uL, 0.14 mmol). After stirring the mixture at ambient temperature for 6 hr, DMSO (0.5 mL) was added and the mixture was purified by preparative HPLC. The pure fractions were combined and lyophilized to give *cis*-2,6-dichloro-*N*-{2-[4-(4-dimethylamino-quinazolin-2-ylamino)-cyclohexyl]-ethyl}-benzamide trifluoro-acetic acid (17.6 mg, 29%) as a white solid.

ESI MS *m/e* 486 *M* + *H*<sup>+</sup>; <sup>1</sup>H NMR (400 MHz, DMSO-*d*<sub>6</sub>) δ 11.93 (brs, 1 H), 8.26 (t, *J* = 5.2 Hz, 1 H), 8.14 (d, *J* = 8.0 Hz, 1 H), 7.95 (brs, 1 H), 7.76 (t, *J* = 8.4 Hz, 1 H), 7.52-7.31 (m, 5 H), 4.15 (m, 1 H), 3.45 (b, 6 H), 3.29 (m, 2 H), 1.76-1.31 (m, 11 H).

## Example 2338



*cis*-*N*<sup>2</sup>-[4-(2-Ethoxy-benzylamino)-cyclohexylmethyl]-*N*<sup>4</sup>,*N*<sup>4</sup>-dimethyl-quinazoline-2,4-diamine ditrifluoro-acetic acid

**Step A: Synthesis of *cis*-(4-aminomethyl-cyclohexyl)-carbamic acid tert-butyl ester.**

To a solution of *cis*-(4-carbamoyl-cyclohexyl)-carbamic acid *tert*-butyl ester obtained in step B of example 2332 (9.68 g, 40 mmol) in THF (100 mL) was added a solution of 1 M BH<sub>3</sub> in THF (80 mL, 80 mmol) over 30 min. The mixture was stirred at reflux for 2 hr. After cooling the reaction mixture to ambient temperature, 1 M aqueous sodium hydroxide was carefully added. The solvents were removed under reduced pressure and the aqueous layer was extracted with CH<sub>2</sub>Cl<sub>2</sub> (twice). The organic layer was dried over sodium sulfate and concentrated under reduced pressure to give *cis*-(4-aminomethyl-cyclohexyl)-carbamic acid *tert*-butyl ester as colorless oil (5.16 g, 57%). ESI MS *m/e* 229 M + H<sup>+</sup>; <sup>1</sup>H NMR (400 MHz, DMSO-*d*<sub>6</sub>) δ 6.67 (d, *J* = 6.8 Hz, 1 H), 3.43 (m, 1 H), 2.41 (d, *J* = 6.4 Hz, 2 H) 1.49-1.22 (m, 18 H).

**Step B: Synthesis of *cis*-{4-[(4-dimethylamino-quinazolin-2-ylamino)-methyl]-cyclohexyl}-carbamic acid *tert*-butyl ester.**

A mixture of *cis*-(4-aminomethyl-cyclohexyl)-carbamic acid *tert*-butyl ester (1.14 g, 5 mmol), (2-chloro-quinazoline-4-yl)-dimethyl-amine obtained in step B of example 1 (1.035 g, 5 mmol), and triethylamine (1.5 mL, 11 mmol) in 2-propanol (2.5 mL) was heated at 170 °C for 35 min using a Smith Microwave Synthesizer. The mixture was concentrated and the residue was purified by column chromatography (silica gel, CH<sub>2</sub>Cl<sub>2</sub> to 10% 2 M NH<sub>3</sub>/MeOH in CH<sub>2</sub>Cl<sub>2</sub>) to give *cis*-{4-[(4-dimethylamino-quinazolin-2-ylamino)-methyl]-cyclohexyl}-carbamic acid *tert*-butyl ester (1.28 g, 80%) as a white solid.

ESI MS *m/e* 400 M + H<sup>+</sup>; <sup>1</sup>H NMR (400 MHz, DMSO-*d*<sub>6</sub>) δ 8.04-7.06 (m, 4 H), 6.77 (d, *J* = 6.0 Hz, 1 H), 3.40-3.16 (m, 9 H), 1.70-1.37 (m, 18 H).

**Step C: Synthesis of *cis*-*N*<sup>2</sup>-(4-amino-cyclohexylmethyl)-*N*<sup>4</sup>,*N*<sup>4</sup>-dimethyl-quinazoline-2,4-diamine.**

A solution of *cis*-{4-[(4-dimethylamino-quinazolin-2-ylamino)-methyl]-cyclohexyl}-carbamic acid *tert*-butyl ester (1.2 g, 3 mmol) in 50% TFA in CH<sub>2</sub>Cl<sub>2</sub> (20 mL) was stirred at ambient temperature. After 30 minutes, the mixture was concentrated and the residue was diluted with 1 M aqueous sodium hydroxide. The aqueous layer was extracted with CH<sub>2</sub>Cl<sub>2</sub> (twice). The combined organic layer was dried over Na<sub>2</sub>SO<sub>4</sub>, filtered and concentrated to give *cis*-*N*<sup>2</sup>-(4-amino-cyclohexylmethyl)-*N*<sup>4</sup>,*N*<sup>4</sup>-dimethyl-quinazoline-2,4-diamine (0.88 g, 98%) as a white solid.

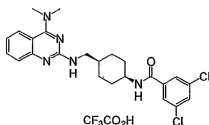
ESI MS  $m/e$  300  $M + H^+$ ;  $^1H$  NMR (400 MHz, DMSO- $d_6$ )  $\delta$  7.85 (d,  $J = 7.6$  Hz, 1 H), 7.47 (t,  $J = 6.8$  Hz, 1 H), 7.27 (brs, 1 H), 7.0 (t,  $J = 7.2$  Hz, 1 H), 6.66 (brs, 1 H), 3.33-3.14 (m, 9 H), 1.69-1.48 (m, 9 H).

**Step D: Synthesis of *cis*- $N^2$ -[4-(2-ethoxy-benzylamino)-cyclohexylmethyl]- $N^4$ , $N^4$ -dimethyl-quinazoline-2,4-diamine ditrifluoro-acetic acid.**

A solution of *cis*- $N^2$ -(4-amino-cyclohexylmethyl)- $N^4$ , $N^4$ -dimethyl-quinazoline-2,4-diamine (30 mg, 0.1 mmol) and 2-ethoxy benzaldehyde (15 mg, 0.1 mmol) in MeOH (1 mL) was stirred at ambient temperature. After 3 hr, NaBH(OAc)<sub>3</sub> (85 mg, 0.4 mmol) was added and the mixture was stirred at ambient temperature for overnight. The resulting mixture was quenched with 50% DMSO in water (2 mL) and the solution was purified by preparative HPLC. The pure fractions were combined and lyophilized to give *cis*- $N^2$ -[4-(2-ethoxy-benzylamino)-cyclohexylmethyl]- $N^4$ , $N^4$ -dimethyl-quinazoline-2,4-diamine ditrifluoro-acetic acid (33 mg, 50%) as a white solid.

ESI MS  $m/e$  434  $M + H^+$ ;  $^1H$  NMR (400 MHz, DMSO- $d_6$ )  $\delta$  13.03 (brs, 1 H), 8.79 (brs, 1 H), 8.49 (m, 2 H), 8.15 (d,  $J = 8.4$  Hz, 1 H), 7.77 (t,  $J = 7.6$  Hz, 1 H), 7.40-7.33 (m, 4 H), 7.07 (d,  $J = 7.6$  Hz, 1 H), 6.99 (t,  $J = 7.2$  Hz, 1 H), 4.11-4.06 (m, 4 H), 3.47-3.41 (m, 8 H), 3.15 (m, 1 H), 1.90-1.60 (m, 9 H), 1.37 (t,  $J = 7.2$  Hz, 3 H).

**Example 2339**



*cis*-3,5-Dichloro- $N$ -{4-[(4-dimethylamino-quinazolin-2-ylamino)-methyl]-cyclohexyl}-benzamide trifluoro-acetic acid

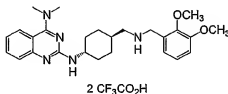
**Step A: Synthesis of *cis*-3,5-dichloro- $N$ -{4-[(4-dimethylamino-quinazolin-2-ylamino)-methyl]-cyclohexyl}-benzamide trifluoro-acetic acid.**

A solution of *cis*- $N^2$ -(4-amino-cyclohexylmethyl)- $N^4$ , $N^4$ -dimethyl-quinazoline-2,4-

diamine (30 mg, 0.1 mmol) and 3,5-dichlorobenzoylchloride (20.9 mg, 0.1 mmol) and pyridine (12  $\mu$ L, 0.25 mmol) in DMSO (1 mL) was stirred at ambient temperature for overnight. The mixture was purified by preparative HPLC. The pure fractions were combined and lyophilized to give *cis*-3,5-dichloro-*N*-{4-[(4-dimethylamino-quinazolin-2-ylamino)-methyl]-cyclohexyl}-benzamide trifluoro-acetic acid.( 18 mg , 31%) as a white solid.

ESI MS  $m/e$  472  $M + H^+$ ;  $^1H$  NMR (400 MHz, DMSO- $d_6$ )  $\delta$  12.13 (brs, 1 H), 8.34 (d,  $J$  = 7.2 Hz, 1 H), 8.15 (d,  $J$  = 8.8 Hz, 1 H), 8.06 (brs, 1 H), 7.82-7.73 (m, 4 H), 7.45 (d,  $J$  = 7.6 Hz, 1 H), 7.36 (t,  $J$  = 7.6 Hz, 1 H), 3.9 (m, 1 H), 3.47-3.25 (m, 8 H), 1.83-1.56 (m, 9 H).

#### Example 2340



*trans*-*N*<sup>2</sup>-{4-[(2,3-Dimethoxy-benzylamino)-methyl]-cyclohexyl}-*N*<sup>4</sup>,*N*<sup>4</sup>-dimethyl-quinazoline-2,4-diamine ditrifluoro-acetic acid

#### Step A: Synthesis of *trans*-4-(*tert*-butoxycarbonylamino-methyl)-cyclohexanecarboxylic acid.

To a solution of *trans*-4-amino-cyclohexanecarboxylic acid (37.7 g, 0.24 mol) in a mixture of dioxane (250 ml) and water (200 ml) cooled in an ice bath were added 1 M aqueous sodium hydroxide (10.07 g, 0.25 mol) and (Boc)<sub>2</sub>O (57.6 g, 0.26 mol). The reaction mixture was stirred at ambient temperature. After 3 hr, the mixture was concentrated and the residue was dissolved in water. The aqueous layer was washed with Et<sub>2</sub>O (3 times). The aqueous layer was cooled in an ice bath and acidified with 1 M aqueous HCl (pH = 2) and the resulting white precipitate was dried to give *trans*-4-(*tert*-butoxycarbonylamino-methyl)-cyclohexanecarboxylic acid (47.4 g, 76.8%) as a white solid.

ESI MS  $m/e$  258  $M + H^+$ ;  $^1H$  NMR (400 MHz, CDCl<sub>3</sub>)  $\delta$  11.95 (brs, 1 H), 6.79 (t,  $J$  = 6.0 Hz, 1 H), 2.76 (t,  $J$  = 6.0 Hz, 2 H), 2.11 (m, 1 H), 1.87 (m, 2 H), 1.69 (m, 2 H), 1.36 (s,

9 H), 1.27 (m, 3 H), 0.9 (m, 2 H).

**Step B: Synthesis of *trans*-[4-(*tert*-butoxycarbonylamino-methyl)-cyclohexyl]-carbamic acid benzyl ester.**

To a solution of *trans*-4-(*tert*-butoxycarbonylamino-methyl)-cyclohexanecarboxylic acid (46.9 g, 0.18 mol) in benzene (300 mL) were added triethylamine (24.2 g, 0.24 mol) and diphenylphosphoryl azide (55.9 g, 0.20 mol). The reaction mixture was stirred at 80 °C for 1 hr. To the mixture was added benzyl alcohol (25.9 g, 0.24 mol) and stirred at 100 °C for 4 hr. The mixture was subsequently cooled to ambient temperature for overnight, concentrated, and the resulting pale orange solid dissolved in EtOAc. The organic layer was washed with water (three times), concentrated, and the residue was purified by column chromatography (silica gel, 50% EtOAc in hexane) to give *trans*-[4-(*tert*-butoxycarbonylamino-methyl)-cyclohexyl]-carbamic acid benzyl ester (66.7g, 100%) as a white solid.

ESI MS *m/e* 363 *M* + *H*<sup>+</sup>; <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>) δ 7.24-7.23 (m, 5 H), 5.06 (s, 2 H), 4.57 (m, 2 H), 3.44 (brs, 1 H), 2.97 (t, *J* = 6.4 Hz, 2 H), 2.04 (m, 2 H), 1.79 (m, 2 H), 1.43 (s, 9 H), 1.08-0.76 (m, 5 H).

**Step C: Synthesis of *trans*-(4-amino-cyclohexylmethyl)-carbamic acid *tert*-butyl ester.**

To a solution of *trans*-[4-(*tert*-butoxycarbonylamino-methyl)-cyclohexyl]-carbamic acid benzyl ester (5.32 g, 0.015 mol) in EtOH (200 mL) was added 10% Pd/C (50 mg). The mixture was stirred at ambient temperature under hydrogen atmosphere for 4 hr. The resulting mixture was filtered through a pad of celite and concentrated. The residue was purified by column chromatography (silica gel, 3% 2 M NH<sub>3</sub>/MeOH in CH<sub>2</sub>Cl<sub>2</sub>) to give *trans*-(4-amino-cyclohexylmethyl)-carbamic acid *tert*-butyl ester as a colorless solid (3.197 g, 95.4%).

ESI MS *m/e* 229 *M* + *H*<sup>+</sup>; <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>) δ 8.44 (brs, 1 H), 4.59 (b, 1 H), 2.96 (m, 2 H), 2.08 (m, 2 H), 1.83 (m, 2 H), 1.43 (s, 9 H), 1.08 (m, 5 H).

**Step D: Synthesis of *trans*-*N*<sup>2</sup>-(4-aminomethyl-cyclohexyl)-*N*<sup>6</sup>,*N*<sup>6</sup>-dimethyl-quinazoline-2,4-diamine ditrifluoro-acetic acid**

A mixture of *trans*-(4-amino-cyclohexylmethyl)-carbamic acid *tert*-butyl ester

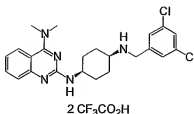
(0.24 g, 1 mmol) and (2-chloro-quinazolin-4-yl)-dimethyl-amine obtained in step B of example 1 (0.32 g, 1.4 mmol) in 2-propanol (5 mL) was heated to 170 °C for 30 min using a Smith Microwave Synthesizer. This procedure was repeated 19 times. The reaction mixtures were combined and purified by column chromatography (silica gel) to give 1.13 g of a yellow solid. The yellow solid was dissolved in 50% TFA in CH<sub>2</sub>Cl<sub>2</sub> (20 mL) and the mixture was stirred at ambient temperature. After 10 hours, the mixture was concentrated and the residue was purified by preparative HPLC. The pure fractions were combined and lyophilized to give *trans*-*N*<sup>2</sup>-(4-aminomethyl-cyclohexyl)-*N*<sup>4</sup>,*N*<sup>4</sup>-dimethyl-quinazoline-2,4-diamine ditrifluoro-acetic acid (0.49 g, 5%) as a white solid.

ESI MS *m/e* 300 M + H<sup>+</sup>; <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>) δ 9.16 (d, *J* = 5.6 Hz, 1 H), 8.11 (m, 2 H), 7.86 (d, *J* = 8.0 Hz, 1 H), 7.51 (t, *J* = 7.6 Hz, 1 H), 7.41 (d, *J* = 8.0 Hz, 1 H), 7.18 (t, *J* = 6.8 Hz, 1 H), 3.8 (brs, 1 H), 3.47 (s, 6 H), 2.10 (m, 2 H), 1.92 (m, 2 H), 1.42-1.12 (m, 5 H).

**Step E: Synthesis of *trans*-*N*<sup>2</sup>-{4-[(2,3-dimethoxy-benzylamino)-methyl]-cyclohexyl}-*N*<sup>4</sup>,*N*<sup>4</sup>-dimethyl-quinazoline-2,4-diamine ditrifluoro-acetic acid.**

A mixture of 2,3-dimethoxy benzaldehyde (15 mg, 0.09 mmol), *trans*-*N*<sup>2</sup>-(4-aminomethyl-cyclohexyl)-*N*<sup>4</sup>,*N*<sup>4</sup>-dimethyl-quinazoline-2,4-diamine ditrifluoro-acetic acid (28 mg, 0.053 mmol), NaBH(OAc)<sub>3</sub> (76 mg, 0.36 mmol), and MeOH (2 mL) was heated at 100 °C for 40 seconds using a Smith Microwave Synthesizer. The resulting mixture was purified by preparative HPLC. The pure fractions were combined and lyophilized to give *trans*-*N*<sup>2</sup>-{4-[(2,3-dimethoxy-benzylamino)-methyl]-cyclohexyl}-*N*<sup>4</sup>,*N*<sup>4</sup>-dimethyl-quinazoline-2,4-diamine ditrifluoro-acetic acid (10.2 mg, 28 %).

ESI MS *m/e* 450 M + H<sup>+</sup>; <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>) δ 9.68 (d, *J* = 6.0 Hz, 1 H), 9.41 (brs, 1 H), 7.85 (d, *J* = 7.6 Hz, 1 H), 7.52 (t, *J* = 7.2 Hz, 1 H), 7.46 (d, *J* = 8.0 Hz, 1 H), 7.19 (t, *J* = 7.2 Hz, 1 H), 7.09 (t, *J* = 8.0 Hz, 1 H), 6.98 (d, *J* = 7.2 Hz, 1 H), 6.90 (d, *J* = 7.6 Hz, 1 H), 4.16 (s, 2 H), 3.96 (s, 3 H), 3.87 (s, 3 H), 3.75 (m, 1 H), 3.47 (m, 6 H), 2.80 (m, 2 H), 2.11 (m, 2 H), 1.86 (m, 2 H), 1.48-1.50 (m, 5 H).

**Example 2341**

***cis*-N<sup>2</sup>-[4-(3,5-Dichloro-benzylamino)-cyclohexyl]-N<sup>4</sup>,N<sup>4</sup>-dimethyl-quinazoline-2,4-diamine ditrifluoro-acetic acid**

**Step A: Synthesis of *cis*-(4-*tert*-butoxycarbonylamino-cyclohexyl)-carbamic acid benzyl ester.**

To a suspension of *cis*-4-*tert*-butoxycarbonylamino-cyclohexanecarboxylic acid (50.0 g, 206 mmol) in benzene were added triethylamine (26.9 g, 266 mmol) and phosphorazidic acid diphenyl ester (62.2 g, 226 mmol). The reaction mixture was stirred at 80°C for 1 hr. Benzyl alcohol (31.4 g, 290 mmol) was added and the mixture was stirred at reflux for 24 hr. The reaction mixture was concentrated and the residue was dissolved in EtOAc and H<sub>2</sub>O. The organic layer was separated and the aqueous layer was extracted with EtOAc (twice). The combined organic layer was dried over MgSO<sub>4</sub>, filtered, concentrated, and purified by flash chromatography (silica gel, 30% EtOAc in hexane) to give *cis*-(4-*tert*-butoxycarbonylamino-cyclohexyl)-carbamic acid benzyl ester (54.1 g, 76%) as a colorless oil.

ESI MS *m/e* 349 M + H<sup>+</sup>; <sup>1</sup>H NMR (400 MHz, DMSO-*d*<sub>6</sub>) δ 7.34-7.28 (m, 5 H), 7.12 (d, *J* = 5.6 Hz, 1 H), 6.62 (brs, 1 H), 4.98 (s, 2 H), 3.39-3.37 (m, 2 H), 1.60-1.45 (m, 8 H), 1.37 (s, 9 H).

**Step B: Synthesis of *cis*-(4-amino-cyclohexyl)-carbamic acid *tert*-butyl ester.**

Using the procedure for the step C of example 2340, the title compound was obtained.

ESI MS *m/e* 215 M + H<sup>+</sup>; <sup>1</sup>H NMR (400 MHz, DMSO-*d*<sub>6</sub>) δ 6.60 (d, *J* = 6.0 Hz, 1 H), 3.30-3.28 (m, 1 H), 2.74 (s, 1 H), 1.59-1.51 (m, 2 H), 1.45-1.37 (m, 15 H).

**Step C: Synthesis of *cis*-[4-(4-dimethylamino-quinazolin-2-ylamino)-cyclohexyl]-**



**carbamic acid *tert*-butyl ester.**

A solution of *cis*-(4-amino-cyclohexyl)-carbamic acid *tert*-butyl ester (0.5 g, 2.3 mmol), (2-chloro-quinazolin-4-yl)-dimethyl-amine obtained in step B in example 1 (0.53, 2.6 mmol), diisopropylethylamine (1.22 mL, 7.0 mmol) and 2-propanol (1.0 mL) was heated using a Smith Microwave Synthesizer at 170 °C for 1 hour. This reaction procedure was repeated 39 more times and the resulting reaction mixtures were combined. The mixture was concentrated and the residue was purified by column chromatography (silica gel, 2% to 4% 2 M NH<sub>3</sub>/MeOH in CH<sub>2</sub>Cl<sub>2</sub>) to give *cis*-[4-(4-dimethylamino-quinazolin-2-ylamino)-cyclohexyl]-carbamic acid *tert*-butyl ester (22.1 g, 0.057 mol, 61%) as a colorless oil.

ESI MS *m/e* 386 M + H<sup>+</sup>; <sup>1</sup>H NMR (400 MHz, DMSO-*d*<sub>6</sub>) δ 7.85 (d, *J* = 8.0 Hz, 1 H), 7.47 (t, *J* = 8.4 Hz, 1 H), 7.27 (d, *J* = 8.0 Hz, 1 H), 7.00 (t, *J* = 7.6 Hz, 1 H), 6.60 (brs, 1 H), 6.18 (brs, 1 H), 3.89-3.88 (m, 1 H), 3.39 (brs, 1 H), 3.19 (s, 6 H), 1.77-1.71 (m, 2 H), 1.68-1.52 (m, 6 H), 1.38 (s, 9 H).

**Step D: Synthesis of *cis*-N<sup>2</sup>-(4-amino-cyclohexyl)-N<sup>4</sup>,N<sup>4</sup>-dimethyl-quinazolin-2,4-diamine.**

Using the procedure for the step C of example 2338, the title compound was obtained.

ESI MS *m/e* 386 M + H<sup>+</sup>; <sup>1</sup>H NMR (400 MHz, DMSO-*d*<sub>6</sub>) δ 7.84 (d, *J* = 8.4 Hz, 1 H), 7.45 (t, *J* = 6.8 Hz, 1 H), 7.26 (d, *J* = 8.4 Hz, 1 H), 6.99 (t, *J* = 7.6 Hz, 1 H), 6.20 (brs, 1 H), 3.90-3.89 (m, 1 H), 3.18 (s, 6 H), 2.79 (s, 1 H), 1.74-1.71 (m, 2 H), 1.57-1.41 (m, 8 H).

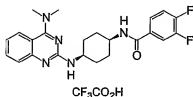
**Step E: Synthesis of *cis*-N<sup>2</sup>-[4-(3,5-dichloro-benzylamino)-cyclohexyl]-N<sup>4</sup>,N<sup>4</sup>-dimethyl-quinazoline-2,4-diamine ditrifluoro-acetic acid.**

To a solution of *cis*-N<sup>2</sup>-(4-amino-cyclohexyl)-N<sup>4</sup>,N<sup>4</sup>-dimethyl-quinazolin-2,4-diamine (31.4 mg, 0.11 mmol) in MeOH (0.5 mL) was added 3,5-dichlorobenzaldehyde (17.5 mg, 0.10 mmol). The mixture was stirred at ambient temperature for 0.5 hr and sodium triacetoxyborohydride (85 mg, 0.40mmol) was added. The mixture was stirred for overnight and the reaction was quenched with 50% DMSO in water (1.0 mL). The mixture was purified by preparative HPLC. The pure fractions were combined and lyophilized to give *cis*-N<sup>2</sup>-[4-(3,5-dichloro-benzylamino)-cyclohexyl]-N<sup>4</sup>,N<sup>4</sup>-dimethyl-quinazoline-2,4-diamine ditrifluoro-acetic acid (23 mg, 0.041 mmol, 37%) as a white

solid.

ESI MS  $m/e$  444  $M + H^+$ ;  $^1H$  NMR (400 MHz, DMSO- $d_6$ )  $\delta$  13.55 (s, 1 H), 8.90 (brs, 3 H), 8.17 (d,  $J = 8.0$  Hz, 1 H), 7.79 (t, 7.6 Hz, 1 H), 7.68 (s, 1 H), 7.61 (s, 2 H), 7.41 (d,  $J = 7.6$  Hz, 1 H), 7.36 (t,  $J = 7.6$  Hz, 1 H), 4.23 (s, 2 H), 4.07 (s, 1 H), 3.48 (s, 6 H), 2.00-1.92 (m, 4 H), 1.82-1.74 (m, 4 H).

### Example 2342



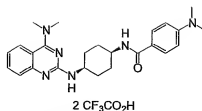
***cis*-N-[4-(4-Dimethylamino-quinazolin-2-ylamino)-cyclohexyl]-3,4-difluorobenzamide trifluoro-acetic acid.**

**Step A: Synthesis of *cis*-N-[4-(4-dimethylamino-quinazolin-2-ylamino)-cyclohexyl]-3,4-difluorobenzamide trifluoro-acetic acid.**

Using the procedure for the step A of example 2333, the title compound was obtained.

ESI MS  $m/e$  426  $M + H^+$ ;  $^1H$  NMR (400 MHz, DMSO- $d_6$ )  $\delta$  12.46 (brs, 1 H), 8.36 (s, 1 H), 8.15 (d,  $J = 8.0$  Hz, 1 H), 7.97 (brs, 1 H), 7.94-7.89 (m, 1 H), 7.77-7.73 (m, 2 H), 7.56-7.49 (m, 1 H), 7.41 (brs, 1 H), 7.36 (t,  $J = 7.6$  Hz, 1 H), 4.07 (m, 1 H), 3.87 (m, 1 H), 3.47 (brs, 6 H), 1.89 (m, 2 H), 1.74 (m, 6 H).

## Example 2343



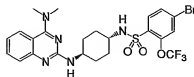
***cis*-4-Dimethylamino-*N*-[4-(4-dimethylamino-quinazolin-2-ylamino)-cyclohexyl]-benzamide ditrifluoro-acetic acid**

**Step A: Synthesis of *cis*-4-dimethylamino-*N*-[4-(4-dimethylamino-quinazolin-2-ylamino)-cyclohexyl]-benzamide ditrifluoro-acetic acid.**

To a solution of 4-dimethylaminobenzoic acid (16.5 mg, 0.10 mmol) in DMF (0.5 mL) were added HATU (45.6 mg, 0.12 mmol), diisopropylethylamine (34.8  $\mu$ L, 0.20 mmol), and *cis*-*N*<sup>2</sup>-(4-amino-cyclohexyl)-*N*<sup>4</sup>,*N*<sup>4</sup>-dimethyl-quinazolin-2,4-diamine obtained in step D of example 2341 (28.5 mg, 0.10 mmol) and stirred at ambient temperature for overnight. The resulting mixture was diluted with DMSO (0.5 mL) and purified by preparative HPLC. The pure fractions combined and lyophilized to give *cis*-4-dimethylamino-*N*-[4-(4-dimethylamino-quinazolin-2-ylamino)-cyclohexyl]-benzamide ditrifluoro-acetic acid (34.1 mg, 0.052 mmol, 52%) as a white solid.

ESI MS  $m/e$  433 M + H<sup>+</sup>; <sup>1</sup>H NMR (400 MHz, DMSO-*d*<sub>6</sub>)  $\delta$  12.73 (s, 1 H), 8.34 (s, 1 H), 8.16 (d,  $J$  = 8.0 Hz, 1 H), 7.78-7.70 (m, 4 H), 7.43 (d,  $J$  = 7.6 Hz, 1 H), 7.35 (t,  $J$  = 8.0 Hz, 1 H), 6.67 (d,  $J$  = 8.8 Hz, 2 H), 4.05 (m, 1 H), 3.86 (m, 1 H), 3.47 (s, 6 H), 2.95 (s, 3 H), 2.53 (s, 3 H), 1.91 (m, 2 H), 1.75-1.72 (m, 6 H).

## Example 2344



***trans*-4-Bromo-*N*-[4-(4-dimethylamino-quinazolin-2-ylamino)-cyclohexyl]-2-trifluoromethoxy-benzenesulfonamide**

**Step A: Synthesis of *trans*-(4-amino-cyclohexyl)-carbamic acid *tert*-butyl ester.**

To a solution of *trans*-1,4-diamino-cyclohexane (10 g, 0.088 mol) in 1,4-dioxane (400 mL) was added a solution of (Boc)<sub>2</sub>O (4.78 g, 0.022 mol) in 1,4-dioxane (100 mL) over 30 min. The mixture was stirred at ambient temperature for overnight and then the dioxane was removed in vacuo. The resulting precipitate was dissolved in H<sub>2</sub>O (500 mL) and left to sit for 1 hour. During this time, the di-Boc-protected diamino-cyclohexane fell out as a white crystalline precipitate. This was subsequently filtered from the aqueous solvent. The aqueous layer was extracted with EtOAc (three times). The organic layers were combined and washed with H<sub>2</sub>O. The organic layer was dried over MgSO<sub>4</sub> and concentrated to give *trans*-(4-amino-cyclohexyl)-carbamic acid *tert*-butyl ester (4 g, 0.019 mol, 85%).

ESI MS *m/e* 215 M + H<sup>+</sup>; <sup>1</sup>H NMR (400 MHz, DMSO-*d*<sub>6</sub>) δ 6.63 (d, *J* = 8.0 Hz, 1 H), 3.11-3.09 (m, 1 H), 2.44-2.37 (m, 1 H), 1.70-1.67 (m, 4 H), 1.41-1.31 (m, 11 H), 1.20-0.95 (m, 4 H).

**Step B: Synthesis of *trans*-[4-(4-bromo-2-trifluoromethoxy-benzenesulfonylamino)-cyclohexyl]-carbamic acid *tert*-butyl ester.**

To a solution of *trans*-(4-amino-cyclohexyl)-carbamic acid *tert*-butyl ester (1 g, 0.0047 mol) in CH<sub>2</sub>Cl<sub>2</sub> were added diisopropylethylamine (1.63 mL, 0.0093 mol) and 4-bromo-2-trifluoromethoxy-benzenesulfonyl chloride (1.03 mL, 0.0051 mol). The reaction mixture was stirred at ambient temperature for 1 hr and then washed with water. The aqueous layer was extracted with CH<sub>2</sub>Cl<sub>2</sub> (twice), the organic layers were combined, dried over MgSO<sub>4</sub>, and concentrated. The resulting precipitate was recrystallized with CH<sub>2</sub>Cl<sub>2</sub> and hexanes to give *trans*-[4-(4-bromo-2-trifluoromethoxy-benzenesulfonylamino)-cyclohexyl]-carbamic acid *tert*-butyl ester (2.39 g, 0.0046 mol, 99%).

ESI MS *m/e* 517 M + H<sup>+</sup>; <sup>1</sup>H NMR (400 MHz, DMSO-*d*<sub>6</sub>) δ 7.99 (d, *J* = 7.6 Hz, 1 H), 7.85 (d, *J* = 8.0 Hz, 1 H), 7.79-7.77 (m, 1 H), 6.67 (d, *J* = 8.0 Hz, 1 H), 3.14-2.94 (m, 2 H), 1.70-1.60 (m, 4 H), 1.34 (s, 9 H), 1.30-1.18 (m, 2 H), 1.14-1.03 (m, 2 H).

**Step C: Synthesis of *trans*-*N*-(4-amino-cyclohexyl)-4-bromo-2-trifluoromethoxy-benzenesulfonamide.**

Using the procedure for the step C of example 2338, the title compound was obtained.

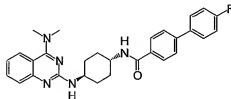
ESI MS  $m/e$  417/419  $M + H^+$ ;  $^1H$  NMR (400 MHz, DMSO- $d_6$ )  $\delta$  7.85 (d,  $J = 8.4$  Hz, 1 H), 7.79-7.76 (m, 3 H), 3.32 (brs, 2 H), 3.03-2.95 (m, 1 H), 2.41-2.36 (m, 1 H), 1.67-1.57 (m, 4 H), 1.28-1.18 (m, 2 H), 0.99-0.89 (m, 2 H).

**Step D: Synthesis of *trans*-4-bromo-*N*-[4-(4-dimethylamino-quinazolin-2-ylamino)-cyclohexyl]-2-trifluoromethoxy-benzenesulfonamide.**

To a solution of *trans*-*N*-(4-amino-cyclohexyl)-4-bromo-2-trifluoromethoxy-benzenesulfonamide (100 mg, 0.24 mmol) in 2-propanol (0.5 mL) was added (2-chloro-quinazolin-4-yl)-dimethyl-amine obtained in step B of example 1 (54.7 mg, 0.26 mmol). The mixture was heated using a Smith Microwave Synthesizer at 170 °C for 15 min. The mixture was concentrated and the residue was purified by chromatography (2% to 4% 2 M  $NH_3/MeOH$  in  $CH_2Cl_2$ ) to give *trans*-4-bromo-*N*-[4-(4-dimethylamino-quinazolin-2-ylamino)-cyclohexyl]-2-trifluoromethoxy-benzenesulfonamide (42 mg, 0.71 mmol, 30%) as a white solid.

ESI MS  $m/e$  588/590  $M + H^+$ ;  $^1H$  NMR (400 MHz, DMSO- $d_6$ )  $\delta$  8.02 (d,  $J = 7.6$  Hz, 1 H), 7.88 (d,  $J = 8.4$  Hz, 1 H), 7.82-7.77 (m, 3 H), 7.45-7.41 (m, 1 H), 7.25-7.41 (m, 1 H), 6.99 (t,  $J = 7.2$  Hz, 1 H), 6.37 (brs, 1 H), 3.68-3.67 (m, 1 H), 3.16 (s, 6 H), 3.09-3.02 (m, 1 H), 1.89-1.86 (m, 2 H), 1.69-1.67 (m, 2 H), 1.40-1.17 (m, 4 H).

**Example 2345**



*trans*-4'-Fluoro-biphenyl-4-carboxylic acid [4-(4-dimethylamino-quinazolin-2-ylamino)-cyclohexyl]-amide.

**Step A: Synthesis of 4'-fluoro-biphenyl-4-carboxylic acid.**

To a solution of 4-bromobenzoic acid (5 g, 0.025 mol) in THF (150 mL) under an

atmosphere of argon were added tetrakis(triphenylphosphine) palladium(0) (862 mg, 0.75 mmol), 2 M aqueous  $\text{Na}_2\text{CO}_3$  (30 mL), and a solution 4-fluorophenylboronic acid (3.48 g, 0.025 mol) in a minimal amount of ethanol (~10 mL). The resulting reaction mixture was stirred at reflux under an argon atmosphere for overnight. The reaction mixture was cooled to ambient temperature and acidified with addition of 1 M HCl aqueous. The aqueous layer was extracted with  $\text{Et}_2\text{O}$  (three times). The organic layers were combined, dried over  $\text{MgSO}_4$ , filtered and concentrated. The resulting precipitate was crystallized in  $\text{Et}_2\text{O}$  and hexane to give 4'-fluoro-biphenyl-4-carboxylic acid (4.4 g, 0.020 mol, 82%) as a white solid.

$^1\text{H}$  NMR (400 MHz,  $\text{DMSO-d}_6$ )  $\delta$  12.96 (s, 1 H), 8.00-7.98 (m, 2 H), 7.78-7.75 (m, 4 H), 7.34-7.31 (m, 2 H).

**Step B: Synthesis of *trans*-[4-(4-dimethylamino-quinazolin-2-ylamino)-cyclohexyl]-carbamic acid *tert*-butyl ester.**

Using the procedure for the step D of example 2344, the title compound was obtained.

ESI MS  $m/e$  386  $\text{M} + \text{H}^+$ ;  $^1\text{H}$  NMR (400 MHz,  $\text{DMSO-d}_6$ )  $\delta$  7.83 (d,  $J = 8.0$  Hz, 1 H), 7.46 (t,  $J = 6.8$  Hz, 1 H), 7.27-7.25 (m, 1 H), 6.99 (t,  $J = 7.2$  Hz, 1 H), 6.71 (d,  $J = 8.4$  Hz, 1 H), 6.38 (brs, 1 H), 3.72 (m, 1 H), 3.17 (s, 6 H), 1.92-1.90 (m, 2 H), 1.79-1.76 (m, 2 H), 1.37 (s, 9 H), 1.34-1.23 (m, 4 H).

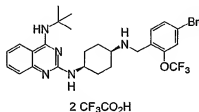
**Step C: Synthesis of *trans*-4'-fluoro-biphenyl-4-carboxylic acid [4-(4-dimethylamino-quinazolin-2-ylamino)-cyclohexyl]-amide.**

To a solution of *trans*-[4-(4-dimethylamino-quinazolin-2-ylamino)-cyclohexyl]-carbamic acid *tert*-butyl ester (0.76 g, 0.20 mmol) in  $\text{CH}_2\text{Cl}_2$  (20 mL) was added TFA (304  $\mu\text{L}$ , 0.39 mmol). The solution was stirred at ambient temperature for 4 hr. The resulting mixture was concentrated and the residue was dissolved in  $\text{CH}_2\text{Cl}_2$ . The organic layer was washed with a dilute aqueous NaOH and aqueous  $\text{NaHCO}_3$  solution. The aqueous layer was extracted with  $\text{CH}_2\text{Cl}_2$  (twice) and the organic layers combined, dried over  $\text{MgSO}_4$ , and concentrated. To a solution of the residue (0.1 g) and 4'-fluoro-biphenyl-4-carboxylic acid (76 mg, 0.35 mmol) in  $\text{CH}_2\text{Cl}_2$  were added HOAt (62 mg, 0.46 mmol), WSC•HCl (87 mg, 0.46 mmol), and diisopropylethylamine (31  $\mu\text{L}$ , 0.18 mmol). The mixture was stirred for 1 hr at ambient temperature and the reaction was quenched with

water. The aqueous layer was extracted with  $\text{CH}_2\text{Cl}_2$  (twice). The organic layers were combined, dried over  $\text{MgSO}_4$ , concentrated and the residue purified by column chromatography (silica gel, 2% to 4% 2 M  $\text{NH}_3/\text{MeOH}$  in  $\text{CH}_2\text{Cl}_2$ ) to give *trans*-4'-fluoro-biphenyl-4-carboxylic acid [4-(4-dimethylamino-quinazolin-2-ylamino)-cyclohexyl]-amide (35 mg, 0.072, 21%) as a white solid.

ESI MS  $m/e$  484  $M + H^+$ ;  $^1\text{H}$  NMR (400 MHz,  $\text{DMSO}-d_6$ )  $\delta$  8.30 (brs, 1 H), 8.12 (brs, 2 H), 7.92 (d,  $J = 8.4$  Hz, 2 H), 7.77-7.72 (m, 5 H), 7.44 (brs, 1 H), 7.34-7.28 (m, 3 H), 3.82 (brs, 2 H), 3.47 (brs, 6 H), 2.04 (m, 2 H), 1.94 (m, 2 H), 1.54-1.48 (m, 4 H).

### Example 2346



*cis*- $N^2$ -[4-(4-Bromo-2-trifluoromethoxy-benzylamino)-cyclohexyl]- $N^4$ -*tert*-butyl-quinazoline-2,4-diamine ditrifluoro-acetic acid

#### Step A: Synthesis of *tert*-butyl-(2-chloro-quinazolin-4-yl)-amine.

To a solution of 2,4-dichloro-quinazoline obtained in step B of example 1 (4 g, 20 mmol) in THF (50 mL) were added *tert*-butyl amine (2.15 mL, 20.5 mmol) and diisopropylethylamine (3.5 mL, 21 mmol). The mixture was stirred at ambient temperature for 2 hr. The mixture was concentrated and the residue was dissolved in EtOAc. The organic layer was washed with water, dried over  $\text{Na}_2\text{SO}_4$ , and filtered. The mixture was concentrated to give *tert*-butyl-(2-chloro-quinazolin-4-yl)-amine as a white solid (3 g, 64%).

ESI MS  $m/e$  236  $M + H^+$ ;  $^1\text{H}$  NMR (400 MHz,  $\text{DMSO}-d_6$ )  $\delta$  8.40 (d,  $J = 8.4$  Hz, 1 H), 7.75-7.36 (m, 2 H), 7.58 (d,  $J = 8.4$  Hz, 1 H), 7.48 (t,  $J = 7.2$  Hz, 1 H), 1.52 (s, 9 H).

#### Step B: Synthesis of *cis*- $N^2$ -(4-amino-cyclohexyl)- $N^4$ -*tert*-butyl-quinazoline-2,4-diamine.

To a suspension of *cis*-(4-amino-cyclohexyl)-carbamic acid *tert*-butyl ester (122

mg, 0.57 mmol) in 2-propanol (2 mL) were added *tert*-butyl-(2-chloro-quinazolin-4-yl)-amine (100 mg, 0.42 mmol) and diisopropylethylamine (180  $\mu$ L, 1 mmol) and the mixture was heated at 170 °C for 1 hr using a Smith Microwave Synthesizer. The resulting solution was concentrated and purified by column chromatography (silica gel, 3% MeOH in  $\text{CH}_2\text{Cl}_2$ ) to give [4-(4-*tert*-butylamino-quinazolin-2-ylamino)-cyclohexyl]-carbamic acid *tert*-butyl ester (112 mg, 65%) as a yellow solid. To a suspension of *cis*-[4-(4-*tert*-butylamino-quinazolin-2-ylamino)-cyclohexyl]-carbamic acid *tert*-butyl ester (95 mg, 0.23 mmol) in  $\text{CH}_2\text{Cl}_2$  (3 mL) was added trifluoroacetic acid (2 mL) dropwise. The reaction mixture was stirred at ambient temperature for 2 hr. The solution was concentrated, alkalinized with saturated aqueous  $\text{NaHCO}_3$ , and 1 M aqueous sodium hydroxide (pH = 9), and the aqueous layer was extracted with  $\text{CH}_2\text{Cl}_2$  (three times). The combined organic layer was dried over  $\text{MgSO}_4$ , filtered, and concentrated. The solid was collected by filtration to give *cis*-*N*<sup>2</sup>-(4-amino-cyclohexyl)-*N*<sup>1</sup>-*tert*-butyl-quinazoline-2,4-diamine (44.6 mg, 53%) as a yellow solid.

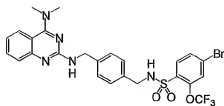
ESI MS  $m/e$  314  $M + H^+$ ;  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  7.48 (t,  $J = 6.8$  Hz, 1 H), 7.38 (m, 2 H), 7.04 (t,  $J = 8.0$  Hz, 1 H), 5.42 (brs, 1 H), 4.15 (m, 1 H), 2.85 (m, 1 H), 1.2-1.9 (m, 17 H).

**Step C: Synthesis of *cis*-*N*<sup>2</sup>-[4-(4-bromo-2-trifluoromethoxy-benzylamino)-cyclohexyl]-*N*<sup>1</sup>-*tert*-butyl-quinazoline-2,4-diamine ditrifluoro-acetic acid.**

Using the procedure for the step C of example 2341, the title compound was obtained.

ESI MS  $m/e$  566  $M + H^+$ ;  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  9.36 (d,  $J = 8.0$  Hz, 1 H), 7.67-7.64 (m, 2 H), 7.53-7.48 (m, 3 H), 7.43 (s, 1 H), 7.33 (m, 1 H), 6.17 (s, 1 H), 4.45 (m, 1 H), 4.28 (s, 2 H), 3.35 (m, 1 H), 2.14-1.6 (m, 17 H).



**Example 2347**

**4-Bromo-*N*-{4-[(4-dimethylamino-quinazolin-2-ylamino)-methyl]-benzyl}-2-trifluoromethoxy-benzenesulfonamide**

**Step A: Synthesis of {4-[(4-dimethylamino-quinazolin-2-ylamino)-methyl]-benzyl}-carbamic acid tert-butyl ester.**

Using the procedure for the step D of example 2330, the title compound was obtained.

ESI MS  $m/e$  377  $M + H^+$ ;  $^1H$  NMR (400 MHz, DMSO- $d_6$ )  $\delta$  8.38 (brs, 1 H), 8.08 (brs, 1 H), 7.70 (brs, 1 H), 7.47 (brs, 1 H), 7.36 (t,  $J = 6.2$  Hz, 1 H), 7.30 (d,  $J = 8.0$  Hz, 3 H), 7.16 (d,  $J = 7.6$  Hz, 2 H), 4.60 (d,  $J = 6.4$  Hz, 2 H), 4.07 (d,  $J = 6.0$  Hz, 2 H), 3.39 (s, 6 H), 1.37 (s, 9 H).

**Step B: Synthesis of *N*<sup>2</sup>-(4-aminomethyl-benzyl)-*N*<sup>4</sup>,*N*<sup>4</sup>-dimethyl-quinazoline-2,4-diamine hydrochloride.**

To a cooled solution of {4-[(4-dimethylamino-quinazolin-2-ylamino)-methyl]-benzyl}-carbamic acid tert-butyl ester (3.90 g, 9.57 mmol) in MeOH was added 1 M HCl in Et<sub>2</sub>O (67.0 ml, 67.0 mmol) and the solution was stirred for overnight. The resulting mixture was concentrated to give *N*<sup>2</sup>-(4-aminomethyl-benzyl)-*N*<sup>4</sup>, *N*<sup>4</sup>-dimethyl-quinazoline-2,4-diamine hydrochloride as a white crystalline solid (3.48 g, 95.6%).

ESI MS  $m/e$  308.2  $M + H^+$ ;  $^1H$  NMR (400 MHz, CD<sub>3</sub>OD)  $\delta$  8.16 (d,  $J = 7.2$  Hz, 1 H), 7.75 (brs, 1 H), 7.48 (m, 5 H), 7.39 (brs, 1 H), 4.76 (s, 2 H), 4.12 (s, 2 H), 3.51 (m, 6 H).

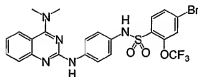
**Step C: Synthesis of 4-bromo-*N*-{4-[(4-dimethylamino-quinazolin-2-ylamino)-methyl]-benzyl}-2-trifluoromethoxy-benzenesulfonamide.**

A solution of *N*<sup>2</sup>-(4-aminomethyl-benzyl)-*N*<sup>4</sup>,*N*<sup>4</sup>-dimethyl-quinazoline-2,4-diamine hydrochloride (50.0 mg, 0.131 mmol), 4-bromo-2-trifluoromethoxy-benzenesulfonyl chloride (53.3 mg, 0.157 mmol) and diisopropylethylamine (91  $\mu$ l, 0.524 mmol) in 2-

propanol (1.5 mL) was stirred at ambient temperature for 2 hr. The resulting mixture was concentrated, and the residue was purified by column chromatography (silica gel, 10% MeOH in  $\text{CH}_2\text{Cl}_2$ ) to give 4-bromo-*N*-{4-[(4-dimethylamino-quinazolin-2-ylamino)-methyl]-benzyl}-2-trifluoromethoxy-benzenesulfonamide as a white crystalline compound (40 mg, 50%).

ESI MS  $m/e$  612  $M + H^+$ ;  $^1\text{H}$  NMR (400 MHz,  $\text{DMSO}-d_6$ )  $\delta$  8.51 (t,  $J = 6.4$  Hz, 1 H), 8.06 (brs, 1 H), 7.76-7.67 (m, 4 H), 7.54-7.41 (m, 2 H), 7.24 (d,  $J = 7.6$  Hz, 3 H), 7.14 (d,  $J = 8.0$  Hz, 2 H), 4.56 (d,  $J = 6.0$  Hz, 2 H), 4.08 (d,  $J = 6.0$  Hz, 2 H), 3.36 (s, 6 H).

### Example 2348



#### 4-bromo-*N*-[4-(4-dimethylamino-quinazolin-2-ylamino)-phenyl]-2-trifluoromethoxy-benzenesulfonamide

##### Step A: Synthesis of (4-amino-phenyl)-carbamic acid *tert*-butyl ester.

Using the procedure for the step A of example 2344, the title compound was obtained.

ESI MS  $m/e$  209  $M + H^+$ ;  $^1\text{H}$  NMR (400 MHz,  $\text{DMSO}-d_6$ )  $\delta$  8.75 (s, 1 H), 7.03 (d,  $J = 7.6$  Hz, 2 H), 6.43 (dt,  $J = 9.5, 2.7$  Hz, 2 H), 4.71 (s, 2 H), 1.43 (s, 9 H).

##### Step B: Synthesis of *N*<sup>2</sup>-(4-amino-phenyl)-*N*<sup>4</sup>,*N*<sup>4</sup>-dimethyl-quinazoline-2,4-diamine hydrochloride.

A mixture of (2-chloro-quinazolin-4-yl)-dimethyl-amine obtained in step B of example 1 (0.5 g, 2.6 mmol) and (4-amino-phenyl)-carbamic acid *tert*-butyl ester (0.5 g, 2.6 mmol) in  $\text{CH}_2\text{Cl}_2$  (2 mL) was heated by Smith Synthesizer at 130 °C for 20 min. The mixture was concentrated to give [4-(4-dimethylamino-quinazolin-2-ylamino)-phenyl]-carbamic acid *tert*-butyl ester as a pale yellow solid (0.86 g, 87%). The reaction was repeated six times, and the total product combined was 8.5 g. To a solution of above product (8.5 g, 22.4 mmol) in MeOH (250 mL) was added 4 M HCl in dioxane (8.4 ml,

33.6 mmol) dropwise, and the mixture was stirred at ambient temperature for overnight. The mixture was concentrated to give *N*<sup>2</sup>-(4-amino-phenyl)-*N*<sup>1</sup>,*N*<sup>4</sup>-dimethyl-quinazoline-2,4-diamine hydrochloride as a pale pink solid (6.2 g, 87.5%).

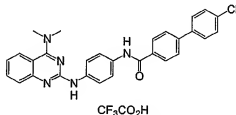
ESI MS *m/e* 280 *M* + *H*<sup>+</sup>; <sup>1</sup>H NMR (400 MHz, D<sub>2</sub>O) δ 7.84 (d, *J* = 8.8 Hz, 1 H), 7.54 (td, *J* = 7.8, 1.2 Hz, 1 H), 7.46 (dt, *J* = 9.5, 2.7 Hz, 2 H), 7.27-7.16 (m, 4 H), 3.35 (b, 3 H), 3.12 (b, 3 H).

**Step C: Synthesis of 4-bromo-*N*-[4-(4-dimethylamino-quinazolin-2-ylamino)-phenyl]-2-trifluoromethoxy-benzenesulfonamide.**

Using the procedure for the step C of example 2347, the title compound was obtained.

ESI MS *m/e* 584 *M* + *H*<sup>+</sup>; <sup>1</sup>H NMR (400 MHz, DMSO-*d*<sub>6</sub>) δ 10.27 (brs, 1 H), 9.14 (brs, 1 H), 7.98 (d, *J* = 8.4 Hz, 1 H), 7.80-7.71 (m, 5 H), 7.60-7.56 (m, 1 H), 7.44 (d, *J* = 8.4 Hz, 1 H), 7.15 (t, *J* = 7.4 Hz, 1 H), 6.95 (d, *J* = 16.8 Hz, 2 H), 9.29 (s, 6 H).

**Example 2349**



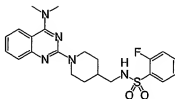
**4'-Chloro-biphenyl-4-carboxylic acid [4-(4-dimethylamino-quinazolin-2-ylamino)-phenyl]-amide trifluoro-acetic acid**

**Synthesis of 4'-chloro-biphenyl-4-carboxylic acid [4-(4-dimethylamino-quinazolin-2-ylamino)-phenyl]-amide trifluoro-acetic acid.**

A solution of *N*<sup>2</sup>-(4-amino-phenyl)-*N*<sup>1</sup>,*N*<sup>4</sup>-dimethyl-quinazoline-2,4-diamine hydrochloride obtained in step B of example 2348 (81.6 mg, 0.258 mmol), 4'-chloro-biphenyl-4-carboxylic acid (50.0 mg, 0.215 mmol), HATU (106 mg, 0.280 mmol), and diisopropylethylamine (150 μL, 0.860 mmol), in CH<sub>2</sub>Cl<sub>2</sub> (2 mL) was stirred at ambient temperature for overnight, and the mixture was concentrated. The residue was purified by HPLC to give 4'-chloro-biphenyl-4-carboxylic acid [4-(4-dimethylamino-quinazolin-2-ylamino)-phenyl]-amide trifluoro-acetic acid as a white solid (10 mg, 9%).

ESI MS  $m/e$  494  $M + H^+$ ;  $^1H$  NMR (400 MHz, DMSO- $d_6$ )  $\delta$  10.33 (s, 1 H), 8.17 (d,  $J = 8.0$  Hz, 1 H), 8.80 (d,  $J = 8.8$  Hz, 2 H), 7.85-7.75 (m, 7 H), 7.63-7.53 (m, 6 H), 7.36 (t,  $J = 7.6$  Hz, 1 H), 3.46 (s, 6 H).

### Example 2350



### *N*-[1-(4-Dimethylamino-quinazolin-2-yl)-piperidin-4-ylmethyl]-2-fluorobenzenesulfonamide

#### Step A: Synthesis of *N*-[1-(4-dimethylamino-quinazolin-2-yl)-piperidin-4-ylmethyl]-2-fluorobenzenesulfonamide.

To a solution of 4-aminomethyl-piperidine-1-carboxylic acid *tert*-butyl ester (60 mg, 0.28 mmol) and diisopropylethylamine (49 mL, 0.28 mmol) in  $CH_2Cl_2$  (2 mL) was added 2-fluorobenzenesulfonyl chloride (54 mg, 0.28 mmol) and the mixture was stirred at ambient temperature for 18 hr. To the resulting mixture was added trifluoroacetic acid (0.70 mL) and stirred at ambient temperature for 18 hr. The reaction mixture was concentrated and neutralized with saturated aqueous  $NaHCO_3$ . The aqueous layer was extracted with EtOAc, and the organic layer was concentrated to give 2-fluoro-*N*-piperidin-4-ylmethyl-benzenesulfonamide as a pale yellow solid. To a solution of above solid (0.076 g, 0.28 mmol) and diisopropylethylamine (0.072 mL, 0.42 mmol) in 2-propanol (3 mL) was added (2-chloro-quinazolin-4-yl)-dimethyl-amine obtained in step B of example 1 (0.044 g, 0.21 mmol) and the resulting mixture was stirred at 100 °C for 18 hr. The mixture was concentrated, and the residue was purified by column chromatography (silica gel, 5% MeOH in  $CH_2Cl_2$ ) to give *N*-[1-(4-dimethylamino-quinazolin-2-yl)-piperidin-4-ylmethyl]-2-fluorobenzenesulfonamide as a pale yellow solid (0.024 g, 26%).

ESI MS  $m/e$  444  $M + H^+$ ;  $^1H$  NMR (400 MHz, DMSO- $d_6$ )  $\delta$  7.98 (m, 1 H), 7.86 (m, 1 H), 7.77 (m, 1 H), 7.67 (m, 1 H), 7.47-7.29 (m, 4 H), 7.02 (m, 1 H), 4.69 (m, 2 H), 3.21 (s, 6 H), 2.76 (m, 4 H), 1.66 (m, 3 H), 1.00 (m, 2 H).

Using the procedure for example 2329 and purification by preparative HPLC, the compounds of example 2351 - 2819 were obtained.

Using the procedure for example 2331 and purification by preparative HPLC, the compounds of example 2820 - 2842 were obtained.

Using the procedure for example 2332, the compounds of example 2843 - 3003 were obtained.

Using the procedure for example 2333, the compounds of example 3004 - 3090 were obtained.

Using the procedure for example 2334, the compounds of example 3091 - 3161 were obtained.

Using the procedure for example 2335 and purification by preparative HPLC, the compounds of example 3162 - 3178 were obtained.

Using the procedure for example 2336, the compounds of example 3179 - 3208 were obtained.

Using the procedure for example 2337, the compounds of example 3209 was obtained.

Using the procedure for example 2338, the compounds of example 3210 - 3225 were obtained.

Using the procedure for example 2339, the compounds of example 3226 - 3228 were obtained.

Using the procedure for example 2340, the compounds of example 3229 - 3231 were obtained.

Using the procedure for example 2341, the compounds of example 3232 - 3393 were obtained.

Using the procedure for example 2342, the compounds of example 3394 - 3472 were obtained.

Using the procedure for example 2343, the compounds of example 3473 - 3527 were obtained.

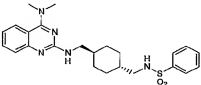
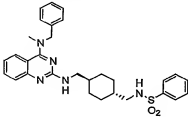
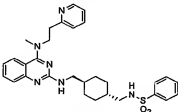
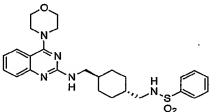
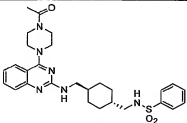
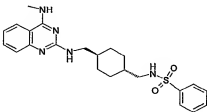
Using the procedure for example 2346, the compounds of example 3528 - 3535 were obtained.

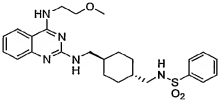
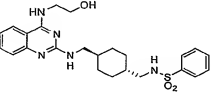
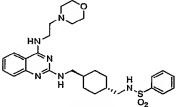
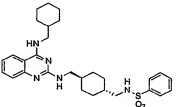
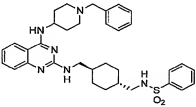
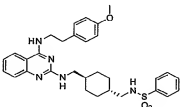
Using the procedure for example 2347 and purification by preparative HPLC, the compounds of example 3536 - 3545 were obtained.

Using the procedure for example 2348 and purification by preparative HPLC, the compounds of example 3546 - 3548 were obtained.

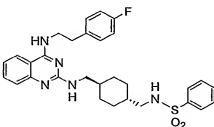
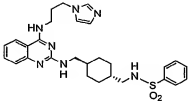
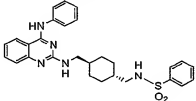
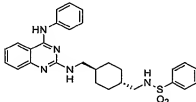
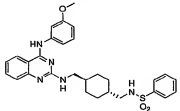
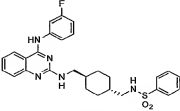
Using the procedure for example 2349, the compounds of example 3549 - 3567 were obtained.

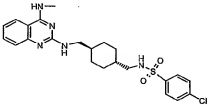
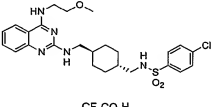
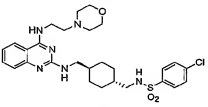
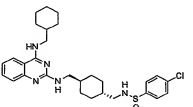
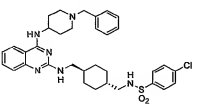
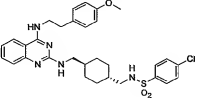
Using the procedure for example 2350 and purification by preparative HPLC, the compounds of example 3568 - 3579 were obtained.

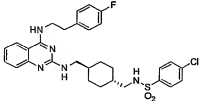
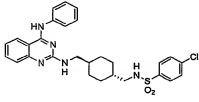
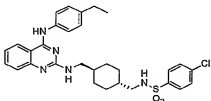
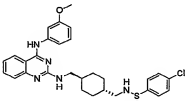
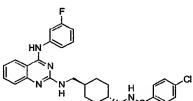
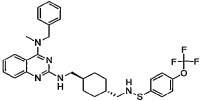
| Example No. | Structure  | ESI-MS        | Retention Time (min) |
|-------------|--|---------------|----------------------|
| 2351        |  <p><math>\text{CF}_3\text{CO}_2\text{H}</math></p>   | 454.0 (M + H) | 3.60                 |
| 2352        |  <p><math>\text{CF}_3\text{CO}_2\text{H}</math></p>   | 530.2 (M + H) | 4.02                 |
| 2353        |  <p><math>2\text{CF}_3\text{CO}_2\text{H}</math></p>  | 545.4 (M + H) | 3.05                 |
| 2354        |  <p><math>\text{CF}_3\text{CO}_2\text{H}</math></p>   | 496.4 (M + H) | 3.49                 |
| 2355        |  <p><math>\text{CF}_3\text{CO}_2\text{H}</math></p>   | 537.4 (M + H) | 3.24                 |
| 2356        |  <p><math>\text{CF}_3\text{CO}_2\text{H}</math></p> | 440.0 (M + H) | 3.47                 |

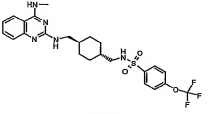
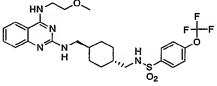
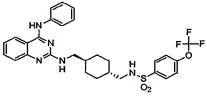
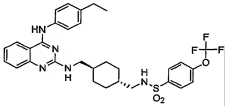
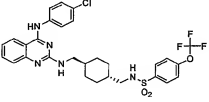
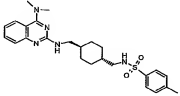
| Example No. | Structure   | ESI-MS        | Retention Time (min) |
|-------------|---|---------------|----------------------|
| 2357        | <br>$\text{CF}_3\text{CO}_2\text{H}$   | 484.4 (M + H) | 3.49                 |
| 2358        | <br>$\text{CF}_3\text{CO}_2\text{H}$   | 470.2 (M + H) | 3.20                 |
| 2359        | <br>$2\text{CF}_3\text{CO}_2\text{H}$  | 539.4 (M + H) | 3.12                 |
| 2360        | <br>$\text{CF}_3\text{CO}_2\text{H}$   | 522.2 (M + H) | 4.22                 |
| 2361        | <br>$2\text{CF}_3\text{CO}_2\text{H}$  | 599.0 (M + H) | 3.48                 |
| 2362        | <br>$\text{CF}_3\text{CO}_2\text{H}$ | 560.2 (M + H) | 3.99                 |

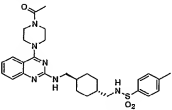
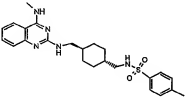
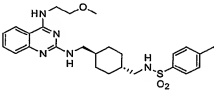
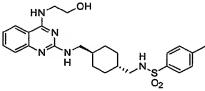
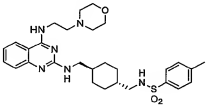
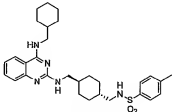


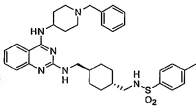
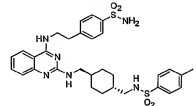
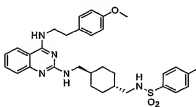
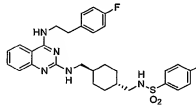
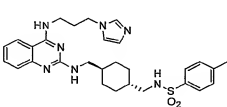
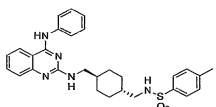
| Example No. | Structure  | ESI-MS        | Retention Time (min) |
|-------------|--|---------------|----------------------|
| 2363        |   | 548.4 (M + H) | 4.06                 |
| 2364        |  <p>2CF<sub>3</sub>CO<sub>2</sub>H</p>  | 534.0 (M + H) | 3.11                 |
| 2365        |  <p>CF<sub>3</sub>CO<sub>2</sub>H</p>   | 502.4 (M + H) | 3.81                 |
| 2366        |  <p>CF<sub>3</sub>CO<sub>2</sub>H</p>   | 530.2 (M + H) | 4.04                 |
| 2367        |  <p>CF<sub>3</sub>CO<sub>2</sub>H</p>   | 532.4 (M + H) | 3.85                 |
| 2368        |  <p>CF<sub>3</sub>CO<sub>2</sub>H</p> | 520.2 (M + H) | 3.86                 |

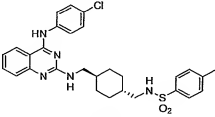
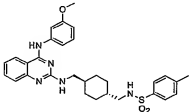
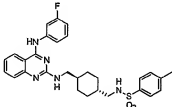
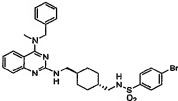
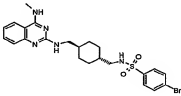
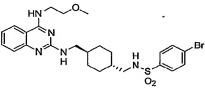
| Example No. | Structure  | ESI-MS        | Retention Time (min) |
|-------------|--|---------------|----------------------|
| 2369        |  <p>CF<sub>3</sub>CO<sub>2</sub>H</p>   | 474.2 (M + H) | 3.72                 |
| 2370        |  <p>CF<sub>3</sub>CO<sub>2</sub>H</p>   | 518.2 (M + H) | 3.71                 |
| 2371        |  <p>2CF<sub>3</sub>CO<sub>2</sub>H</p>  | 573.2 (M + H) | 3.15                 |
| 2372        |  <p>CF<sub>3</sub>CO<sub>2</sub>H</p>   | 556.2 (M + H) | 4.38                 |
| 2373        |  <p>2CF<sub>3</sub>CO<sub>2</sub>H</p>  | 633.4 (M + H) | 3.48                 |
| 2374        |  <p>CF<sub>3</sub>CO<sub>2</sub>H</p> | 594.2 (M + H) | 4.23                 |

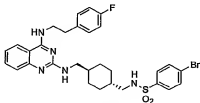
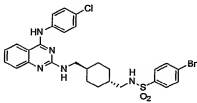
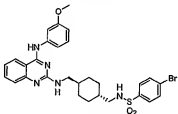
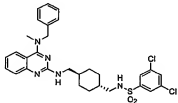
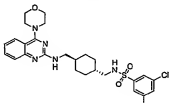
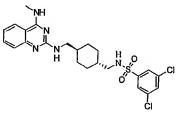
| Example No. | Structure  | ESI-MS        | Retention Time (min) |
|-------------|--|---------------|----------------------|
| 2375        |  <p>CF<sub>3</sub>CO<sub>2</sub>H</p>   | 582.4 (M + H) | 4.26                 |
| 2376        |  <p>CF<sub>3</sub>CO<sub>2</sub>H</p>   | 536.2 (M + H) | 4.06                 |
| 2377        |  <p>CF<sub>3</sub>CO<sub>2</sub>H</p>   | 564.2 (M + H) | 4.32                 |
| 2378        |  <p>CF<sub>3</sub>CO<sub>2</sub>H</p>   | 566.4 (M + H) | 4.11                 |
| 2379        |  <p>CF<sub>3</sub>CO<sub>2</sub>H</p>   | 554.2 (M + H) | 4.10                 |
| 2380        |  <p>CF<sub>3</sub>CO<sub>2</sub>H</p> | 614.2 (M + H) | 4.26                 |

| Example No. | Structure  | ESI-MS        | Retention Time (min) |
|-------------|--|---------------|----------------------|
| 2381        |  <p>CF<sub>3</sub>CO<sub>2</sub>H</p>   | 524.4 (M + H) | 3.87                 |
| 2382        |  <p>CF<sub>3</sub>CO<sub>2</sub>H</p>   | 568.2 (M + H) | 3.87                 |
| 2383        |  <p>CF<sub>3</sub>CO<sub>2</sub>H</p>   | 586.2 (M + H) | 4.18                 |
| 2384        |  <p>CF<sub>3</sub>CO<sub>2</sub>H</p>   | 614.2 (M + H) | 4.45                 |
| 2385        |  <p>CF<sub>3</sub>CO<sub>2</sub>H</p>   | 620.4 (M + H) | 4.32                 |
| 2386        |  <p>CF<sub>3</sub>CO<sub>2</sub>H</p> | 468.2 (M + H) | 3.20                 |

| Example No. | Structure  | ESI-MS        | Retention Time (min) |
|-------------|--|---------------|----------------------|
| 2387        |  <p>CF<sub>3</sub>CO<sub>2</sub>H</p>   | 551.6 (M + H) | 2.82                 |
| 2388        |  <p>CF<sub>3</sub>CO<sub>2</sub>H</p>   | 454.0 (M + H) | 3.06                 |
| 2389        |  <p>CF<sub>3</sub>CO<sub>2</sub>H</p>   | 498.6 (M + H) | 3.10                 |
| 2390        |  <p>CF<sub>3</sub>CO<sub>2</sub>H</p>   | 484.2 (M + H) | 2.76                 |
| 2391        |  <p>2CF<sub>3</sub>CO<sub>2</sub>H</p>  | 553.6 (M + H) | 2.40                 |
| 2392        |  <p>CF<sub>3</sub>CO<sub>2</sub>H</p> | 536.4 (M + H) | 3.77                 |

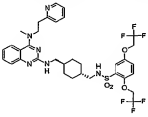
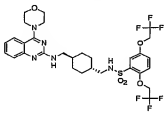
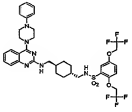
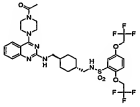
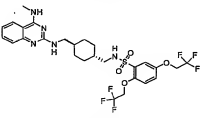
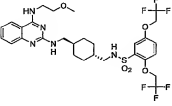
| Example No. | Structure  | ESI-MS        | Retention Time (min) |
|-------------|--|---------------|----------------------|
| 2393        |  <p>2CF<sub>3</sub>CO<sub>2</sub>H</p>  | 613.4 (M + H) | 2.74                 |
| 2394        |  <p>CF<sub>3</sub>CO<sub>2</sub>H</p>   | 623.4 (M + H) | 3.06                 |
| 2395        |  <p>CF<sub>3</sub>CO<sub>2</sub>H</p>   | 574.4 (M + H) | 3.51                 |
| 2396        |  <p>CF<sub>3</sub>CO<sub>2</sub>H</p>   | 562.2 (M + H) | 3.59                 |
| 2397        |  <p>2CF<sub>3</sub>CO<sub>2</sub>H</p>  | 548.6 (M + H) | 2.48                 |
| 2398        |  <p>CF<sub>3</sub>CO<sub>2</sub>H</p> | 516.4 (M + H) | 3.39                 |

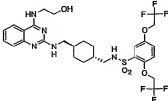
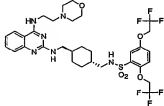
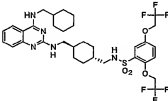
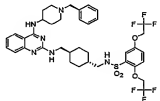
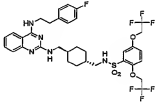
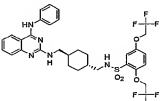
| Example No. | Structure  | ESI-MS        | Retention Time (min) |
|-------------|--|---------------|----------------------|
| 2399        |  <p>CF<sub>3</sub>CO<sub>2</sub>H</p>   | 550.4 (M + H) | 3.56                 |
| 2400        |  <p>CF<sub>3</sub>CO<sub>2</sub>H</p>   | 546.2 (M + H) | 3.38                 |
| 2401        |  <p>CF<sub>3</sub>CO<sub>2</sub>H</p>   | 534.0 (M + H) | 3.43                 |
| 2402        |  <p>CF<sub>3</sub>CO<sub>2</sub>H</p>   | 608.2 (M + H) | 3.75                 |
| 2403        |  <p>CF<sub>3</sub>CO<sub>2</sub>H</p>   | 518 (M + H)   | 3.22                 |
| 2404        |  <p>CF<sub>3</sub>CO<sub>2</sub>H</p> | 562.2 (M + H) | 3.20                 |

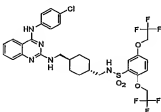
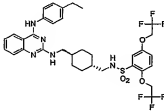
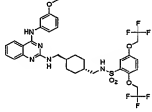
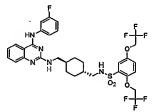
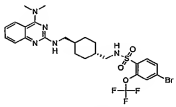
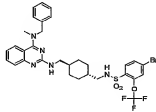
| Example No. | Structure   | ESI-MS        | Retention Time (min) |
|-------------|---|---------------|----------------------|
| 2405        | <br>$\text{CF}_3\text{CO}_2\text{H}$   | 626.0 (M + H) | 3.76                 |
| 2406        | <br>$\text{CF}_3\text{CO}_2\text{H}$   | 614.0 (M + H) | 3.72                 |
| 2407        | <br>$\text{CF}_3\text{CO}_2\text{H}$   | 610.0 (M + H) | 3.57                 |
| 2408        | <br>$\text{CF}_3\text{CO}_2\text{H}$   | 598.2 (M + H) | 3.97                 |
| 2409        | <br>$\text{CF}_3\text{CO}_2\text{H}$   | 564.2 (M + H) | 3.46                 |
| 2410        | <br>$\text{CF}_3\text{CO}_2\text{H}$ | 508.0 (M + H) | 3.44                 |

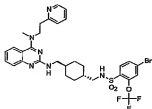
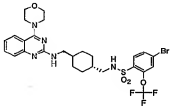
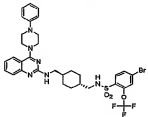
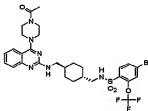
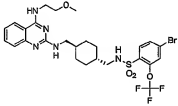
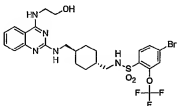


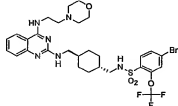
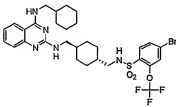
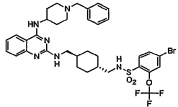
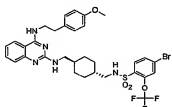
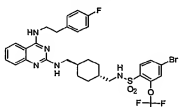
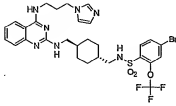
| Example No. | Structure                            | ESI-MS        | Retention Time (min) |
|-------------|--------------------------------------|---------------|----------------------|
| 2411        | <p>CF<sub>3</sub>CO<sub>2</sub>H</p> | 616.2 (M + H) | 3.94                 |
| 2412        | <p>CF<sub>3</sub>CO<sub>2</sub>H</p> | 604.2 (M + H) | 4.51                 |
| 2413        | <p>CF<sub>3</sub>CO<sub>2</sub>H</p> | 600.2 (M + H) | 4.32                 |
| 2414        | <p>CF<sub>3</sub>CO<sub>2</sub>H</p> | 588.0 (M + H) | 4.38                 |
| 2415        | <p>CF<sub>3</sub>CO<sub>2</sub>H</p> | 650.2 (M + H) | 4.20                 |
| 2416        | <p>CF<sub>3</sub>CO<sub>2</sub>H</p> | 726.4 (M + H) | 4.52                 |

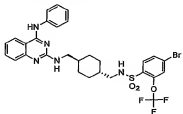
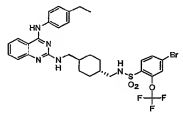
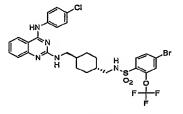
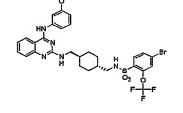
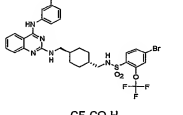
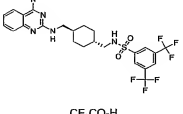
| Example No. | Structure  | ESI-MS        | Retention Time (min) |
|-------------|--|---------------|----------------------|
| 2417        | <br>$2CF_3CO_2H$  | 741.6 (M + H) | 3.59                 |
| 2418        | <br>$CF_3CO_2H$   | 692.2 (M + H) | 4.12                 |
| 2419        | <br>$2CF_3CO_2H$  | 767.6 (M + H) | 4.59                 |
| 2420        | <br>$CF_3CO_2H$   | 733.4 (M + H) | 3.87                 |
| 2421        | <br>$CF_3CO_2H$   | 636.2 (M + H) | 4.08                 |
| 2422        | <br>$CF_3CO_2H$ | 680.2 (M + H) | 4.07                 |

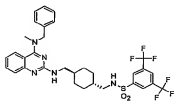
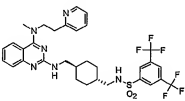
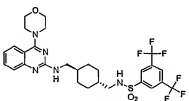
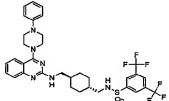
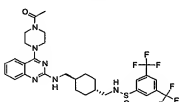
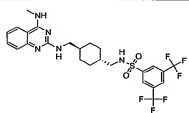
| Example No. | Structure   | ESI-MS        | Retention Time (min) |
|-------------|---|---------------|----------------------|
| 2423        | <br>$\text{CF}_3\text{CO}_2\text{H}$   | 666.0 (M + H) | 3.86                 |
| 2424        | <br>$2\text{CF}_3\text{CO}_2\text{H}$  | 735.4 (M + H) | 3.50                 |
| 2425        | <br>$\text{CF}_3\text{CO}_2\text{H}$   | 718.4 (M + H) | 4.64                 |
| 2426        | <br>$2\text{CF}_3\text{CO}_2\text{H}$  | 795.6 (M + H) | 3.70                 |
| 2427        | <br>$\text{CF}_3\text{CO}_2\text{H}$   | 744.2 (M + H) | 4.43                 |
| 2428        | <br>$\text{CF}_3\text{CO}_2\text{H}$ | 698.0 (M + H) | 4.26                 |

| Example No. | Structure  | ESI-MS        | Retention Time (min) |
|-------------|--|---------------|----------------------|
| 2429        |  <p>CF<sub>3</sub>CO<sub>2</sub>H</p>   | 732.4 (M + H) | 4.37                 |
| 2430        |  <p>CF<sub>3</sub>CO<sub>2</sub>H</p>   | 726.4 (M + H) | 4.52                 |
| 2431        |  <p>CF<sub>3</sub>CO<sub>2</sub>H</p>   | 728.4 (M + H) | 4.36                 |
| 2432        |  <p>CF<sub>3</sub>CO<sub>2</sub>H</p>   | 716.4 (M + H) | 4.32                 |
| 2433        |  <p>CF<sub>3</sub>CO<sub>2</sub>H</p>   | 616.0 (M + H) | 4.22                 |
| 2434        |  <p>CF<sub>3</sub>CO<sub>2</sub>H</p> | 692.0 (M + H) | 4.57                 |

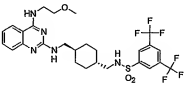
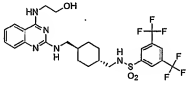
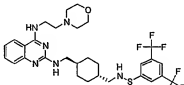
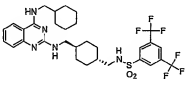
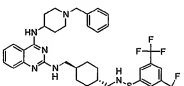
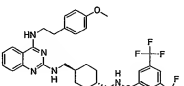
| Example No. | Structure  | ESI-MS        | Retention Time (min) |
|-------------|--|---------------|----------------------|
| 2435        |  <p>2CF<sub>3</sub>CO<sub>2</sub>H</p>  | 707.2 (M + H) | 3.64                 |
| 2436        |  <p>CF<sub>3</sub>CO<sub>2</sub>H</p>   | 658.2 (M + H) | 4.15                 |
| 2437        |  <p>CF<sub>3</sub>CO<sub>2</sub>H</p>   | 733.2 (M + H) | 4.68                 |
| 2438        |  <p>CF<sub>3</sub>CO<sub>2</sub>H</p>   | 699.2 (M + H) | 3.88                 |
| 2439        |  <p>CF<sub>3</sub>CO<sub>2</sub>H</p>   | 646.4 (M + H) | 4.08                 |
| 2440        |  <p>CF<sub>3</sub>CO<sub>2</sub>H</p> | 632.4 (M + H) | 3.86                 |

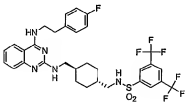
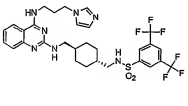
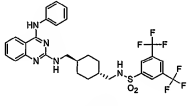
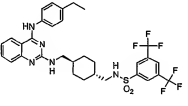
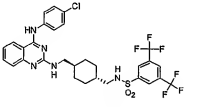
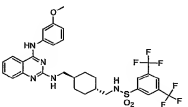
| Example No. | Structure  | ESI-MS        | Retention Time (min) |
|-------------|--|---------------|----------------------|
| 2441        | <br>$2\text{CF}_3\text{CO}_2\text{H}$   | 701.4 (M + H) | 3.51                 |
| 2442        | <br>$\text{CF}_3\text{CO}_2\text{H}$    | 684.2 (M + H) | 4.75                 |
| 2443        | <br>$2\text{CF}_3\text{CO}_2\text{H}$   | 761.2 (M + H) | 3.74                 |
| 2444        | <br>$\text{CF}_3\text{CO}_2\text{H}$    | 722.2 (M + H) | 4.59                 |
| 2445        | <br>$\text{CF}_3\text{CO}_2\text{H}$    | 710.2 (M + H) | 4.60                 |
| 2446        | <br>$2\text{CF}_3\text{CO}_2\text{H}$ | 696.2 (M + H) | 3.53                 |

| Example No. | Structure  | ESI-MS        | Retention Time (min) |
|-------------|--|---------------|----------------------|
| 2447        |  <p>CF<sub>3</sub>CO<sub>2</sub>H</p>   | 664.2 (M + H) | 4.39                 |
| 2448        |  <p>CF<sub>3</sub>CO<sub>2</sub>H</p>   | 692.0 (M + H) | 4.65                 |
| 2449        |  <p>CF<sub>3</sub>CO<sub>2</sub>H</p>   | 698.0 (M + H) | 4.59                 |
| 2450        |  <p>CF<sub>3</sub>CO<sub>2</sub>H</p>   | 694.2 (M + H) | 4.42                 |
| 2451        |  <p>CF<sub>3</sub>CO<sub>2</sub>H</p>  | 682.2 (M + H) | 4.42                 |
| 2452        |  <p>CF<sub>3</sub>CO<sub>2</sub>H</p> | 590.2 (M + H) | 4.28                 |

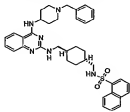
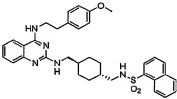
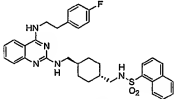
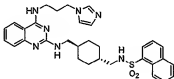
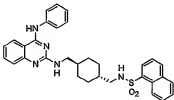
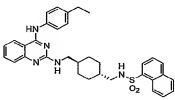
| Example No. | Structure   | ESI-MS        | Retention Time (min) |
|-------------|---|---------------|----------------------|
| 2453        | <br>$\text{CF}_3\text{CO}_2\text{H}$   | 666.2 (M + H) | 4.61                 |
| 2454        | <br>$2\text{CF}_3\text{CO}_2\text{H}$  | 681.2 (M + H) | 3.72                 |
| 2455        | <br>$\text{CF}_3\text{CO}_2\text{H}$   | 632.4 (M + H) | 4.21                 |
| 2456        | <br>$2\text{CF}_3\text{CO}_2\text{H}$  | 707.2 (M + H) | 4.70                 |
| 2457        | <br>$\text{CF}_3\text{CO}_2\text{H}$   | 673.2 (M + H) | 3.94                 |
| 2458        | <br>$\text{CF}_3\text{CO}_2\text{H}$ | 576.2 (M + H) | 4.16                 |

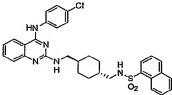
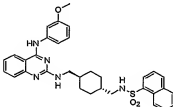
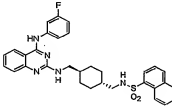
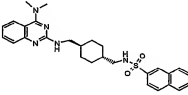
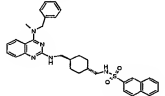
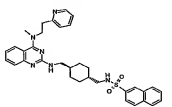


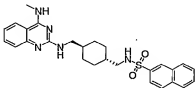
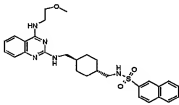
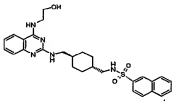
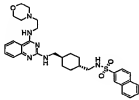
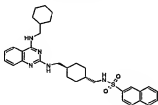
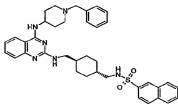
| Example No. | Structure  | ESI-MS        | Retention Time (min) |
|-------------|--|---------------|----------------------|
| 2459        |  <p>CF<sub>3</sub>CO<sub>2</sub>H</p>   | 620.4 (M + H) | 4.19                 |
| 2460        |  <p>CF<sub>3</sub>CO<sub>2</sub>H</p>   | 606.6 (M + H) | 3.94                 |
| 2461        |  <p>2CF<sub>3</sub>CO<sub>2</sub>H</p>  | 675.4 (M + H) | 3.59                 |
| 2462        |  <p>CF<sub>3</sub>CO<sub>2</sub>H</p>   | 658.6 (M + H) | 4.82                 |
| 2463        |  <p>2CF<sub>3</sub>CO<sub>2</sub>H</p>  | 735.4 (M + H) | 3.82                 |
| 2464        |  <p>CF<sub>3</sub>CO<sub>2</sub>H</p> | 696.0 (M + H) | 4.56                 |

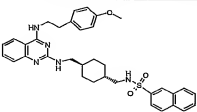
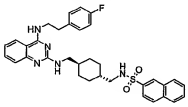
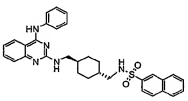
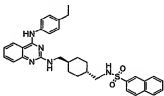
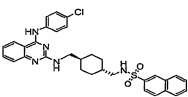
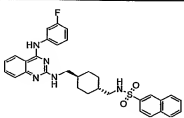
| Example No. | Structure  | ESI-MS        | Retention Time (min) |
|-------------|--|---------------|----------------------|
| 2465        |  <p>CF<sub>3</sub>CO<sub>2</sub>H</p>   | 684.4 (M + H) | 4.61                 |
| 2466        |  <p>2CF<sub>3</sub>CO<sub>2</sub>H</p>  | 670.2 (M + H) | 3.56                 |
| 2467        |  <p>CF<sub>3</sub>CO<sub>2</sub>H</p>   | 638.2 (M + H) | 4.43                 |
| 2468        |  <p>CF<sub>3</sub>CO<sub>2</sub>H</p>   | 666.2 (M + H) | 4.68                 |
| 2469        |  <p>CF<sub>3</sub>CO<sub>2</sub>H</p>   | 672.2 (M + H) | 4.60                 |
| 2470        |  <p>CF<sub>3</sub>CO<sub>2</sub>H</p> | 668.2 (M + H) | 4.44                 |

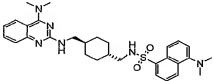
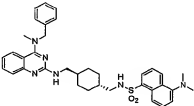
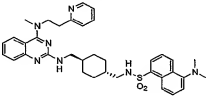
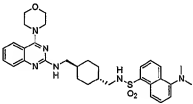
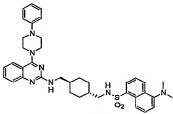
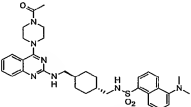


| Example No. | Structure   | ESI-MS        | Retention Time (min) |
|-------------|---|---------------|----------------------|
| 2477        | <br>$2\text{CF}_3\text{CO}_2\text{H}$  | 649.4 (M + H) | 3.50                 |
| 2478        | <br>$\text{CF}_3\text{CO}_2\text{H}$   | 610.4 (M + H) | 4.26                 |
| 2479        | <br>$\text{CF}_3\text{CO}_2\text{H}$   | 598.2 (M + H) | 4.30                 |
| 2480        | <br>$2\text{CF}_3\text{CO}_2\text{H}$  | 584.4 (M + H) | 3.29                 |
| 2481        | <br>$\text{CF}_3\text{CO}_2\text{H}$   | 552.6 (M + H) | 4.11                 |
| 2482        | <br>$\text{CF}_3\text{CO}_2\text{H}$ | 580.6 (M + H) | 4.40                 |

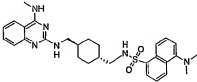
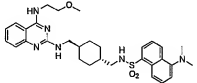
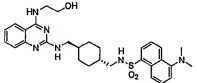
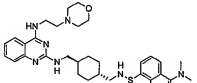
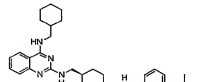
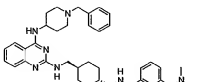
| Example No. | Structure   | ESI-MS        | Retention Time (min) |
|-------------|---|---------------|----------------------|
| 2483        |  <p>CF<sub>3</sub>CO<sub>2</sub>H</p>    | 586.2 (M + H) | 4.30                 |
| 2484        |  <p>CF<sub>3</sub>CO<sub>2</sub>H</p>    | 582.4 (M + H) | 4.14                 |
| 2485        |  <p>CF<sub>3</sub>CO<sub>2</sub>H</p>    | 570.2 (M + H) | 4.14                 |
| 2486        |  <p>CF<sub>3</sub>CO<sub>2</sub>H</p>    | 504.2 (M + H) | 3.94                 |
| 2487        |  <p>CF<sub>3</sub>CO<sub>2</sub>H</p>    | 580.6 (M + H) | 4.34                 |
| 2488        |  <p>2CF<sub>3</sub>CO<sub>2</sub>H</p> | 595.2 (M + H) | 3.41                 |

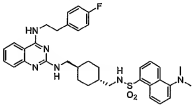
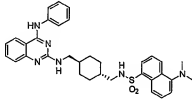
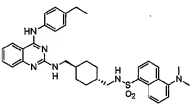
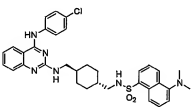
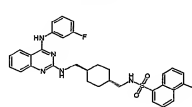
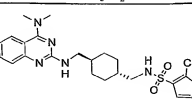
| Example No. | Structure  | ESI-MS        | Retention Time (min) |
|-------------|--|---------------|----------------------|
| 2489        | <br>$\text{CF}_3\text{CO}_2\text{H}$    | 490.2 (M + H) | 3.84                 |
| 2490        | <br>$\text{CF}_3\text{CO}_2\text{H}$    | 534.2 (M + H) | 3.84                 |
| 2491        | <br>$\text{CF}_3\text{CO}_2\text{H}$    | 520.4 (M + H) | 3.60                 |
| 2492        | <br>$2\text{CF}_3\text{CO}_2\text{H}$   | 589.2 (M + H) | 3.29                 |
| 2493        | <br>$\text{CF}_3\text{CO}_2\text{H}$    | 572.4 (M + H) | 4.51                 |
| 2494        | <br>$2\text{CF}_3\text{CO}_2\text{H}$ | 649.4 (M + H) | 3.52                 |

| Example No. | Structure   | ESI-MS      | Retention Time (min) |
|-------------|---|-------------|----------------------|
| 2495        | <br>$\text{CF}_3\text{CO}_2\text{H}$   | 610.2 (M+H) | 4.29                 |
| 2496        | <br>$\text{CF}_3\text{CO}_2\text{H}$   | 598.2 (M+H) | 4.34                 |
| 2497        | <br>$\text{CF}_3\text{CO}_2\text{H}$   | 552.6 (M+H) | 4.13                 |
| 2498        | <br>$\text{CF}_3\text{CO}_2\text{H}$   | 580.6 (M+H) | 4.37                 |
| 2499        | <br>$\text{CF}_3\text{CO}_2\text{H}$   | 586.2 (M+H) | 4.30                 |
| 2500        | <br>$\text{CF}_3\text{CO}_2\text{H}$ | 570.2 (M+H) | 4.18                 |

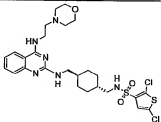
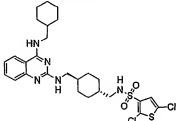
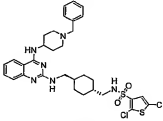
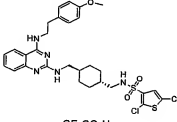
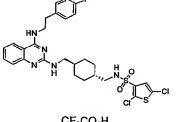
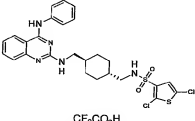
| Example No. | Structure   | ESI-MS        | Retention Time (min) |
|-------------|---|---------------|----------------------|
| 2501        | <br>$2CF_3CO_2H$   | 547.4 (M + H) | 3.69                 |
| 2502        | <br>$2CF_3CO_2H$   | 623.4 (M + H) | 4.10                 |
| 2503        | <br>$3CF_3CO_2H$   | 638.2 (M + H) | 3.20                 |
| 2504        | <br>$2CF_3CO_2H$   | 589.2 (M + H) | 3.62                 |
| 2505        | <br>$3CF_3CO_2H$   | 664.4 (M + H) | 4.25                 |
| 2506        | <br>$2CF_3CO_2H$ | 630.4 (M + H) | 3.35                 |

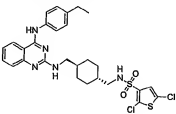
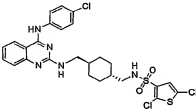
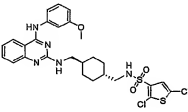
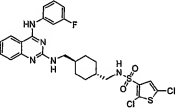
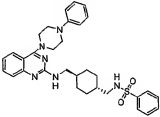
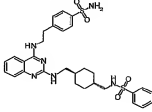


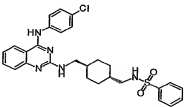
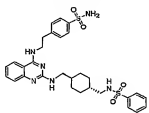
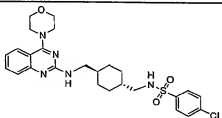
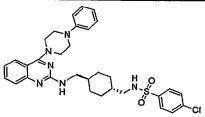
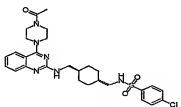
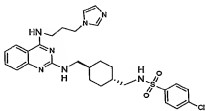
| Example No. | Structure  | ESI-MS        | Retention Time (min) |
|-------------|--|---------------|----------------------|
| 2507        | <br><chem>CC1=CC=C2C(=C1)C(=C(C=C2)S(=O)(=O)NC3CCCCC3C4=NC5=CC=CC=C5N=C4N)C6CCCCC6</chem><br>$2CF_3CO_2H$                               | 533.2 (M + H) | 3.57                 |
| 2508        | <br><chem>COCCNc1nc2ccccc2n1C3CCCCC3C4=NC5=CC=CC=C5N=C4N(S(=O)(=O)NC6=CC=CC=C6C7=CC=CC=C7N(C)C)C8CCCCC8</chem><br>$2CF_3CO_2H$          | 577.6 (M + H) | 3.58                 |
| 2509        | <br><chem>OCCNc1nc2ccccc2n1C3CCCCC3C4=NC5=CC=CC=C5N=C4N(S(=O)(=O)NC6=CC=CC=C6C7=CC=CC=C7N(C)C)C8CCCCC8</chem><br>$2CF_3CO_2H$           | 563.2 (M + H) | 3.28                 |
| 2510        | <br><chem>O=C1CCN(C1)CCNc2nc3ccccc3n2C4CCCCC4C5=NC6=CC=CC=C6N=C5N(S(=O)(=O)NC7=CC=CC=C7C8=CC=CC=C8N(C)C)C9CCCCC9</chem><br>$3CF_3CO_2H$ | 632.6 (M + H) | 3.06                 |
| 2511        | <br><chem>C1CCCCC1Nc2nc3ccccc3n2C4CCCCC4C5=NC6=CC=CC=C6N=C5N(S(=O)(=O)NC7=CC=CC=C7C8=CC=CC=C8N(C)C)C9CCCCC9</chem><br>$2CF_3CO_2H$      | 615.4 (M + H) | 4.30                 |
| 2512        | <br><chem>C1CCCCC1Nc2nc3ccccc3n2C4CCCCC4C5=NC6=CC=CC=C6N=C5N(S(=O)(=O)NC7=CC=CC=C7C8=CC=CC=C8N(C)C)C9CCCCC9</chem><br>$3CF_3CO_2H$    | 692.2 (M + H) | 3.38                 |

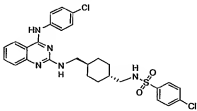
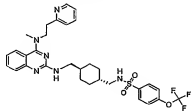
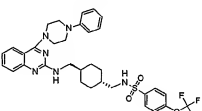
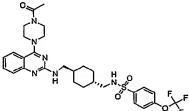
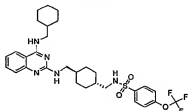
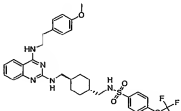
| Example No. | Structure  | ESI-MS        | Retention Time (min) |
|-------------|--|---------------|----------------------|
| 2513        |  <p>2CF<sub>3</sub>CO<sub>2</sub>H</p>  | 641.4 (M + H) | 4.13                 |
| 2514        |  <p>2CF<sub>3</sub>CO<sub>2</sub>H</p>  | 595.4 (M + H) | 3.89                 |
| 2515        |  <p>2CF<sub>3</sub>CO<sub>2</sub>H</p>  | 623.4 (M + H) | 4.20                 |
| 2516        |  <p>2CF<sub>3</sub>CO<sub>2</sub>H</p>  | 629.2 (M + H) | 4.15                 |
| 2517        |  <p>2CF<sub>3</sub>CO<sub>2</sub>H</p>  | 613.2 (M + H) | 4.02                 |
| 2518        |  <p>CF<sub>3</sub>CO<sub>2</sub>H</p> | 528.2 (M + H) | 4.03                 |

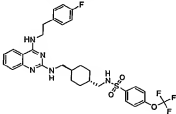
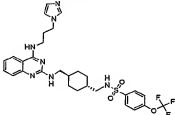
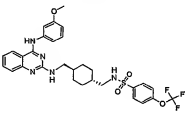
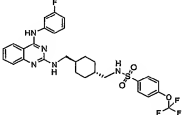
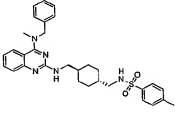
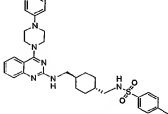
| Example No. | Structure                             | ESI-MS        | Retention Time (min) |
|-------------|---------------------------------------|---------------|----------------------|
| 2519        | <p>CF<sub>3</sub>CO<sub>2</sub>H</p>  | 570.2 (M + H) | 3.96                 |
| 2520        | <p>CF<sub>3</sub>CO<sub>2</sub>H</p>  | 611.0 (M + H) | 3.69                 |
| 2521        | <p>CF<sub>3</sub>CO<sub>2</sub>H</p>  | 514.2 (M + H) | 3.94                 |
| 2522        | <p>2CF<sub>3</sub>CO<sub>2</sub>H</p> | 625.4 (M + H) | 3.94                 |
| 2523        | <p>CF<sub>3</sub>CO<sub>2</sub>H</p>  | 558.2 (M + H) | 3.96                 |
| 2524        | <p>CF<sub>3</sub>CO<sub>2</sub>H</p>  | 544.2 (M + H) | 3.67                 |

| Example No. | Structure  | ESI-MS        | Retention Time (min) |
|-------------|--|---------------|----------------------|
| 2525        | <br>$2CF_3CO_2H$  | 613.2 (M + H) | 3.31                 |
| 2526        | <br>$CF_3CO_2H$   | 596.2 (M + H) | 4.69                 |
| 2527        | <br>$2CF_3CO_2H$  | 673.4 (M + H) | 3.57                 |
| 2528        | <br>$CF_3CO_2H$   | 634.4 (M + H) | 4.41                 |
| 2529        | <br>$CF_3CO_2H$  | 622.2 (M + H) | 4.45                 |
| 2530        | <br>$CF_3CO_2H$ | 576 (M + H)   | 4.25                 |

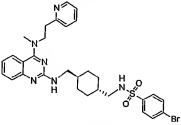
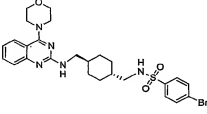
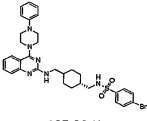
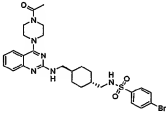
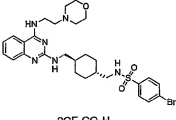
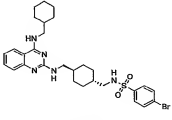
| Example No. | Structure   | ESI-MS        | Retention Time (min) |
|-------------|---|---------------|----------------------|
| 2531        | <br>$\text{CF}_3\text{CO}_2\text{H}$   | 604.4 (M + H) | 4.52                 |
| 2532        | <br>$\text{CF}_3\text{CO}_2\text{H}$   | 610.2 (M + H) | 4.40                 |
| 2533        | <br>$\text{CF}_3\text{CO}_2\text{H}$   | 606.4 (M + H) | 4.29                 |
| 2534        | <br>$\text{CF}_3\text{CO}_2\text{H}$   | 594.2 (M + H) | 4.27                 |
| 2535        | <br>$2\text{CF}_3\text{CO}_2\text{H}$  | 571.8 (M + H) | 4.99                 |
| 2536        | <br>$\text{CF}_3\text{CO}_2\text{H}$ | 609.8 (M + H) | 4.43                 |

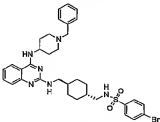
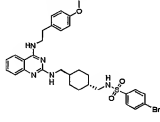
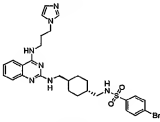
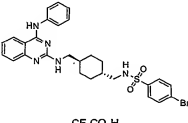
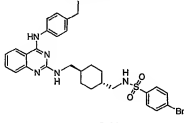
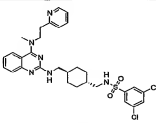
| Example No. | Structure  | ESI-MS        | Retention Time (min) |
|-------------|--|---------------|----------------------|
| 2537        | <br>$\text{CF}_3\text{CO}_2\text{H}$    | 536.4 (M + H) | 4.86                 |
| 2538        | <br>$\text{CF}_3\text{CO}_2\text{H}$    | 564.6 (M + H) | 5.13                 |
| 2539        | <br>$\text{CF}_3\text{CO}_2\text{H}$    | 530.6 (M + H) | 4.65                 |
| 2540        | <br>$2\text{CF}_3\text{CO}_2\text{H}$   | 605.6 (M + H) | 5.21                 |
| 2541        | <br>$\text{CF}_3\text{CO}_2\text{H}$    | 571.6 (M + H) | 4.45                 |
| 2542        | <br>$2\text{CF}_3\text{CO}_2\text{H}$ | 568.8 (M + H) | 4.09                 |

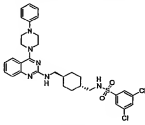
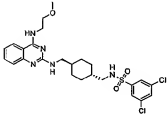
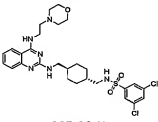
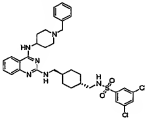
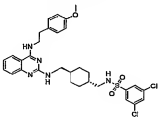
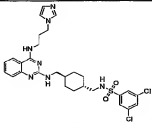
| Example No. | Structure   | ESI-MS        | Retention Time (min) |
|-------------|---|---------------|----------------------|
| 2543        | <br>$\text{CF}_3\text{CO}_2\text{H}$   | 570.6 (M + H) | 5.11                 |
| 2544        | <br>$2\text{CF}_3\text{CO}_2\text{H}$  | 629.6 (M + H) | 4.37                 |
| 2545        | <br>$2\text{CF}_3\text{CO}_2\text{H}$  | 655.6 (M + H) | 5.35                 |
| 2546        | <br>$\text{CF}_3\text{CO}_2\text{H}$   | 621.8 (M + H) | 4.63                 |
| 2547        | <br>$\text{CF}_3\text{CO}_2\text{H}$   | 606.8 (M + H) | 5.45                 |
| 2548        | <br>$\text{CF}_3\text{CO}_2\text{H}$ | 644.6 (M + H) | 5.21                 |

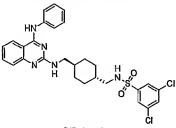
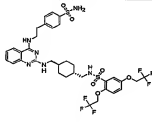
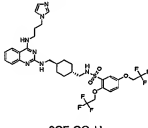
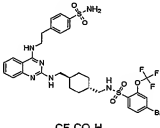
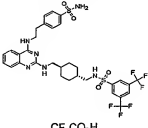
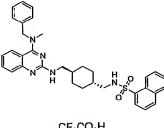
| Example No. | Structure  | ESI-MS        | Retention Time (min) |
|-------------|--|---------------|----------------------|
| 2549        | <br>$\text{CF}_3\text{CO}_2\text{H}$    | 632.6 (M + H) | 5.25                 |
| 2550        | <br>$2\text{CF}_3\text{CO}_2\text{H}$   | 618.6 (M + H) | 4.29                 |
| 2551        | <br>$\text{CF}_3\text{CO}_2\text{H}$    | 616.6 (M + H) | 5.14                 |
| 2552        | <br>$\text{CF}_3\text{CO}_2\text{H}$    | 604.6 (M + H) | 5.13                 |
| 2553        | <br>$\text{CF}_3\text{CO}_2\text{H}$    | 544.6 (M + H) | 5.03                 |
| 2554        | <br>$2\text{CF}_3\text{CO}_2\text{H}$ | 585.6 (M + H) | 5.13                 |

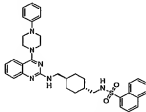
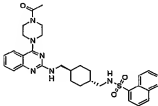
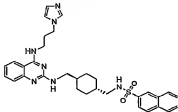
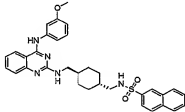
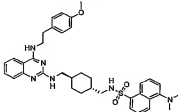
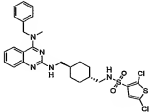


| Example No. | Structure  | ESI-MS        | Retention Time (min) |
|-------------|--|---------------|----------------------|
| 2555        | <br>$2CF_3CO_2H$  | 623.6 (M + H) | 4.25                 |
| 2556        | <br>$CF_3CO_2H$   | 574.6 (M + H) | 4.73                 |
| 2557        | <br>$2CF_3CO_2H$  | 649.0 (M + H) | 5.25                 |
| 2558        | <br>$CF_3CO_2H$   | 615.0 (M + H) | 4.51                 |
| 2559        | <br>$2CF_3CO_2H$ | 617.4 (M + H) | 4.15                 |
| 2560        | <br>$CF_3CO_2H$ | 600.6 (M + H) | 5.37                 |

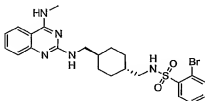
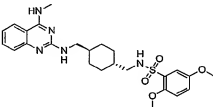
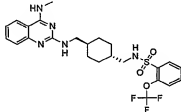
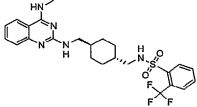
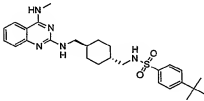
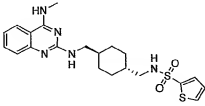
| Example No. | Structure  | ESI-MS        | Retention Time (min) |
|-------------|--|---------------|----------------------|
| 2561        | <br>$2\text{CF}_3\text{CO}_2\text{H}$   | 677.0 (M + H) | 4.45                 |
| 2562        | <br>$\text{CF}_3\text{CO}_2\text{H}$    | 638.6 (M + H) | 5.18                 |
| 2563        | <br>$2\text{CF}_3\text{CO}_2\text{H}$   | 612.6 (M + H) | 4.16                 |
| 2564        | <br>$\text{CF}_3\text{CO}_2\text{H}$    | 580.0 (M + H) | 5.01                 |
| 2565        | <br>$\text{CF}_3\text{CO}_2\text{H}$   | 608.0 (M + H) | 5.26                 |
| 2566        | <br>$2\text{CF}_3\text{CO}_2\text{H}$ | 613.6 (M + H) | 4.44                 |

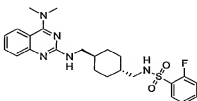
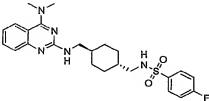
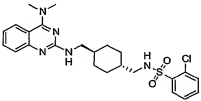
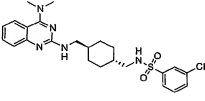
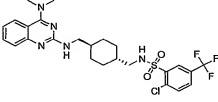
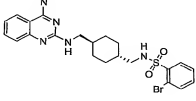
| Example No. | Structure   | ESI-MS        | Retention Time (min) |
|-------------|---|---------------|----------------------|
| 2567        | <br>$2CF_3CO_2H$   | 639.6 (M + H) | 5.48                 |
| 2568        | <br>$CF_3CO_2H$    | 552.6 (M + H) | 4.92                 |
| 2569        | <br>$2CF_3CO_2H$   | 607.8 (M + H) | 4.33                 |
| 2570        | <br>$2CF_3CO_2H$   | 667.4 (M + H) | 4.67                 |
| 2571        | <br>$CF_3CO_2H$    | 628.6 (M + H) | 5.29                 |
| 2572        | <br>$2CF_3CO_2H$ | 602.6 (M + H) | 4.35                 |

| Example No. | Structure  | ESI-MS        | Retention Time (min) |
|-------------|--|---------------|----------------------|
| 2573        |  <p>CF<sub>3</sub>CO<sub>2</sub>H</p>   | 570.6 (M + H) | 5.23                 |
| 2574        |  <p>CF<sub>3</sub>CO<sub>2</sub>H</p>   | 805.4 (M + H) | 4.91                 |
| 2575        |  <p>2CF<sub>3</sub>CO<sub>2</sub>H</p>  | 730.8 (M + H) | 4.47                 |
| 2576        |  <p>CF<sub>3</sub>CO<sub>2</sub>H</p>   | 771.6 (M + H) | 4.93                 |
| 2577        |  <p>CF<sub>3</sub>CO<sub>2</sub>H</p>  | 745.6 (M + H) | 5.01                 |
| 2578        |  <p>CF<sub>3</sub>CO<sub>2</sub>H</p> | 580.8 (M + H) | 5.18                 |

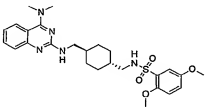
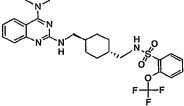
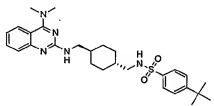
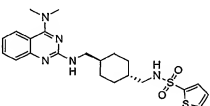
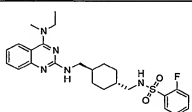
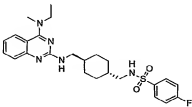
| Example No. | Structure  | ESI-MS        | Retention Time (min) |
|-------------|--|---------------|----------------------|
| 2579        | <br>$2CF_3CO_2H$  | 621.8 (M + H) | 5.27                 |
| 2580        | <br>$CF_3CO_2H$   | 587.6 (M + H) | 4.51                 |
| 2581        | <br>$2CF_3CO_2H$  | 584.6 (M + H) | 4.21                 |
| 2582        | <br>$CF_3CO_2H$   | 582.8 (M + H) | 5.03                 |
| 2583        | <br>$CF_3CO_2H$   | 653.8 (M + H) | 4.90                 |
| 2584        | <br>$CF_3CO_2H$ | 604.6 (M + H) | 5.33                 |

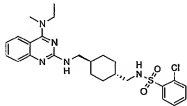
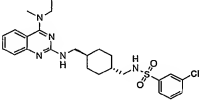
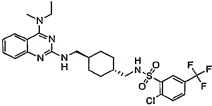
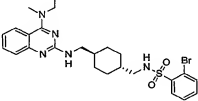
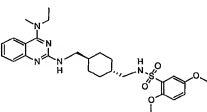
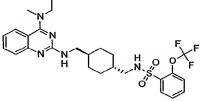


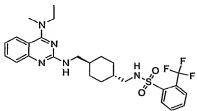
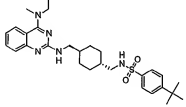
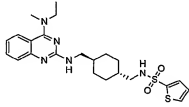
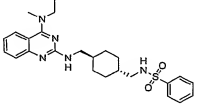
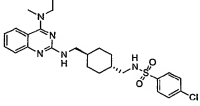
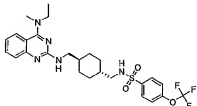
| Example No. | Structure  | ESI-MS        | Retention Time (min) |
|-------------|--|---------------|----------------------|
| 2591        |  <p>CF<sub>3</sub>CO<sub>2</sub>H</p>   | 518.6 (M + H) | 4.51                 |
| 2592        |  <p>CF<sub>3</sub>CO<sub>2</sub>H</p>   | 500.8 (M + H) | 4.33                 |
| 2593        |  <p>CF<sub>3</sub>CO<sub>2</sub>H</p>   | 524.6 (M + H) | 4.61                 |
| 2594        |  <p>CF<sub>3</sub>CO<sub>2</sub>H</p>   | 508.6 (M + H) | 4.57                 |
| 2595        |  <p>CF<sub>3</sub>CO<sub>2</sub>H</p>   | 496.8 (M + H) | 4.87                 |
| 2596        |  <p>CF<sub>3</sub>CO<sub>2</sub>H</p> | 446.8 (M + H) | 4.29                 |

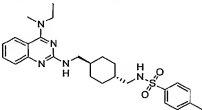
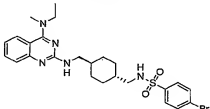
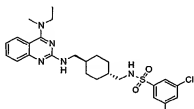
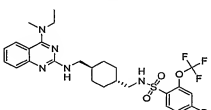
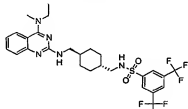
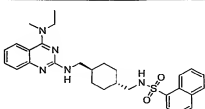
| Example No. | Structure   | ESI-MS        | Retention Time (min) |
|-------------|---|---------------|----------------------|
| 2597        | <br>$\text{CF}_3\text{CO}_2\text{H}$   | 472.8 (M + H) | 4.47                 |
| 2598        | <br>$\text{CF}_3\text{CO}_2\text{H}$   | 472.8 (M + H) | 4.53                 |
| 2599        | <br>$\text{CF}_3\text{CO}_2\text{H}$   | 488.6 (M + H) | 4.55                 |
| 2600        | <br>$\text{CF}_3\text{CO}_2\text{H}$   | 487.6 (M + H) | 4.65                 |
| 2601        | <br>$\text{CF}_3\text{CO}_2\text{H}$   | 556.6 (M + H) | 4.91                 |
| 2602        | <br>$\text{CF}_3\text{CO}_2\text{H}$ | 532.4 (M + H) | 4.61                 |



| Example No. | Structure   | ESI-MS        | Retention Time (min) |
|-------------|---|---------------|----------------------|
| 2603        | <br><chem>CC1=NC2=CC=CC=C2N1N=C3C(=NC(=C3)N(C)C)NS4CCCCC4NS(=O)(=O)c5cc(OC)cc(OC)c5</chem><br>$\text{CF}_3\text{CO}_2\text{H}$   | 514.8 (M + H) | 4.43                 |
| 2604        | <br><chem>CC1=NC2=CC=CC=C2N1N=C3C(=NC(=C3)N(C)C)NS4CCCCC4NS(=O)(=O)c5ccc(cc5)C(F)(F)F</chem><br>$\text{CF}_3\text{CO}_2\text{H}$ | 538.6 (M + H) | 4.80                 |
| 2605        | <br><chem>CC1=NC2=CC=CC=C2N1N=C3C(=NC(=C3)N(C)C)NS4CCCCC4NS(=O)(=O)c5ccc(cc5)C(C)(C)C</chem><br>$\text{CF}_3\text{CO}_2\text{H}$ | 510.6 (M + H) | 5.00                 |
| 2606        | <br><chem>CC1=NC2=CC=CC=C2N1N=C3C(=NC(=C3)N(C)C)NS4CCCCC4NS(=O)(=O)c5ccsc5</chem><br>$\text{CF}_3\text{CO}_2\text{H}$            | 460.6 (M + H) | 4.40                 |
| 2607        | <br><chem>CC1=NC2=CC=CC=C2N1N=C3C(=NC(=C3)N(C)C)NS4CCCCC4NS(=O)(=O)c5ccccc5F</chem><br>$\text{CF}_3\text{CO}_2\text{H}$          | 486.6 (M + H) | 4.60                 |
| 2608        | <br><chem>CC1=NC2=CC=CC=C2N1N=C3C(=NC(=C3)N(C)C)NS4CCCCC4NS(=O)(=O)c5ccc(F)cc5</chem><br>$\text{CF}_3\text{CO}_2\text{H}$      | 484.6 (M + H) | 4.64                 |

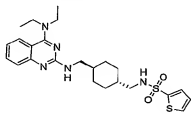
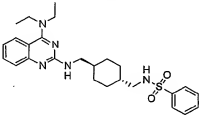
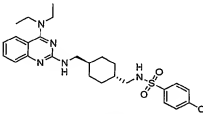
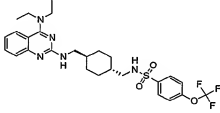
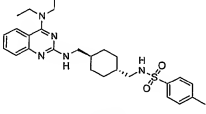
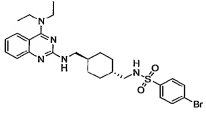
| Example No. | Structure  | ESI-MS        | Retention Time (min) |
|-------------|--|---------------|----------------------|
| 2609        | <br><chem>CC1=NC2=CC=CC=C2N1N=C(NC3=CC=CC=C3S(=O)(=O)N4C=CC(=CC=C4)Cl)CC5CCCCC5</chem><br>$\text{CF}_3\text{CO}_2\text{H}$          | 503.6 (M + H) | 4.74                 |
| 2610        | <br><chem>CC1=NC2=CC=CC=C2N1N=C(NC3=CC=CC=C3S(=O)(=O)N4C=CC(=CC=C4)Cl)CC5CCCCC5</chem><br>$\text{CF}_3\text{CO}_2\text{H}$          | 502.6 (M + H) | 4.86                 |
| 2611        | <br><chem>CC1=NC2=CC=CC=C2N1N=C(NC3=CC=CC=C3S(=O)(=O)N4C=CC(=CC=C4)C(F)(F)F)CC5CCCCC5</chem><br>$\text{CF}_3\text{CO}_2\text{H}$    | 570.8 (M + H) | 5.00                 |
| 2612        | <br><chem>CC1=NC2=CC=CC=C2N1N=C(NC3=CC=CC=C3S(=O)(=O)N4C=CC(=CC=C4)Br)CC5CCCCC5</chem><br>$\text{CF}_3\text{CO}_2\text{H}$          | 546.0 (M + H) | 4.80                 |
| 2613        | <br><chem>CC1=NC2=CC=CC=C2N1N=C(NC3=CC=CC=C3S(=O)(=O)N4C=CC(=CC=C4)OC)CC5CCCCC5</chem><br>$\text{CF}_3\text{CO}_2\text{H}$          | 528.8 (M + H) | 4.63                 |
| 2614        | <br><chem>CC1=NC2=CC=CC=C2N1N=C(NC3=CC=CC=C3S(=O)(=O)N4C=CC(=CC=C4)OC(F)(F)F)CC5CCCCC5</chem><br>$\text{CF}_3\text{CO}_2\text{H}$ | 552.8 (M + H) | 4.90                 |

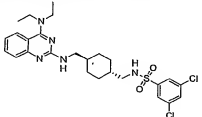
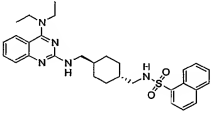
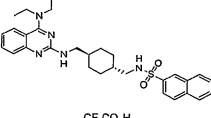
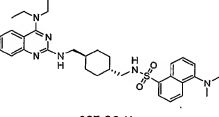
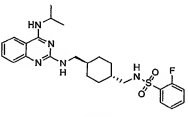
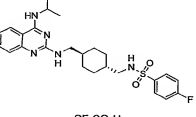
| Example No. | Structure   | ESI-MS        | Retention Time (min) |
|-------------|---|---------------|----------------------|
| 2615        | <br><chem>CCN(C)c1nc2ccccc2n1CNC3CCCCC3NS(=O)(=O)c4cc(F)c(F)cc4</chem><br>$\text{CF}_3\text{CO}_2\text{H}$     | 536.6 (M + H) | 4.82                 |
| 2616        | <br><chem>CCN(C)c1nc2ccccc2n1CNC3CCCCC3NS(=O)(=O)c4ccc(C(C)(C)C)cc4</chem><br>$\text{CF}_3\text{CO}_2\text{H}$ | 524.8 (M + H) | 5.07                 |
| 2617        | <br><chem>CCN(C)c1nc2ccccc2n1CNC3CCCCC3NS(=O)(=O)c4ccsc4</chem><br>$\text{CF}_3\text{CO}_2\text{H}$            | 474.6 (M + H) | 4.55                 |
| 2618        | <br><chem>CCN(C)c1nc2ccccc2n1CNC3CCCCC3NS(=O)(=O)c4ccccc4</chem><br>$\text{CF}_3\text{CO}_2\text{H}$           | 468.4 (M + H) | 4.59                 |
| 2619        | <br><chem>CCN(C)c1nc2ccccc2n1CNC3CCCCC3NS(=O)(=O)c4ccc(Cl)cc4</chem><br>$\text{CF}_3\text{CO}_2\text{H}$       | 502.6 (M + H) | 4.81                 |
| 2620        | <br><chem>CCN(C)c1nc2ccccc2n1CNC3CCCCC3NS(=O)(=O)c4ccc(OC(F)F)cc4</chem><br>$\text{CF}_3\text{CO}_2\text{H}$ | 552.8 (M + H) | 4.94                 |

| Example No. | Structure   | ESI-MS        | Retention Time (min) |
|-------------|---|---------------|----------------------|
| 2621        | <br>$\text{CF}_3\text{CO}_2\text{H}$   | 482.6 (M + H) | 4.73                 |
| 2622        | <br>$\text{CF}_3\text{CO}_2\text{H}$   | 546.6 (M + H) | 4.85                 |
| 2623        | <br>$\text{CF}_3\text{CO}_2\text{H}$   | 536.4 (M + H) | 5.08                 |
| 2624        | <br>$\text{CF}_3\text{CO}_2\text{H}$   | 630.4 (M + H) | 5.11                 |
| 2625        | <br>$\text{CF}_3\text{CO}_2\text{H}$   | 604.6 (M + H) | 5.16                 |
| 2626        | <br>$\text{CF}_3\text{CO}_2\text{H}$ | 518.6 (M + H) | 4.75                 |

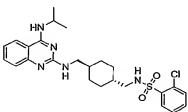
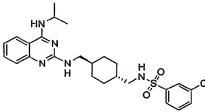
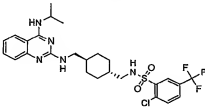
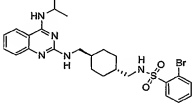
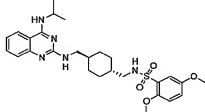
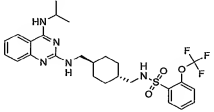


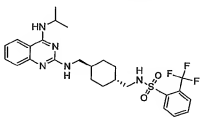
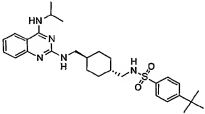
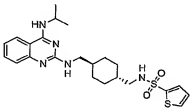
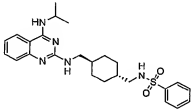
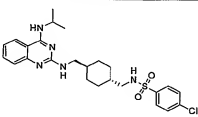
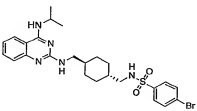


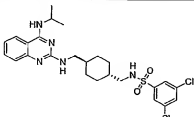
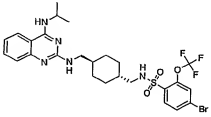
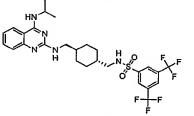
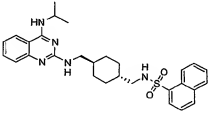
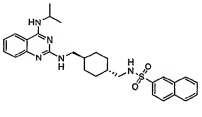
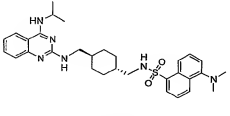
| Example No. | Structure   | ESI-MS        | Retention Time (min) |
|-------------|---|---------------|----------------------|
| 2639        | <br>$\text{CF}_3\text{CO}_2\text{H}$   | 488.6 (M + H) | 4.65                 |
| 2640        | <br>$\text{CF}_3\text{CO}_2\text{H}$   | 482.6 (M + H) | 4.73                 |
| 2641        | <br>$\text{CF}_3\text{CO}_2\text{H}$   | 516.8 (M + H) | 4.97                 |
| 2642        | <br>$\text{CF}_3\text{CO}_2\text{H}$   | 566.6 (M + H) | 5.12                 |
| 2643        | <br>$\text{CF}_3\text{CO}_2\text{H}$   | 496.8 (M + H) | 4.89                 |
| 2644        | <br>$\text{CF}_3\text{CO}_2\text{H}$ | 560.0 (M + H) | 4.98                 |

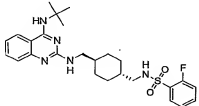
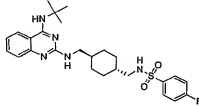
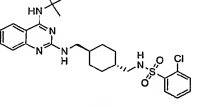
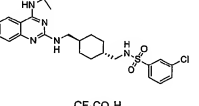
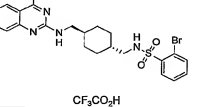
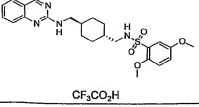
| Example No. | Structure   | ESI-MS        | Retention Time (min) |
|-------------|---|---------------|----------------------|
| 2645        | <br>$\text{CF}_3\text{CO}_2\text{H}$   | 550.6 (M + H) | 5.21                 |
| 2646        | <br>$\text{CF}_3\text{CO}_2\text{H}$   | 532.6 (M + H) | 4.99                 |
| 2647        | <br>$\text{CF}_3\text{CO}_2\text{H}$   | 532.6 (M + H) | 5.03                 |
| 2648        | <br>$2\text{CF}_3\text{CO}_2\text{H}$  | 575.8 (M + H) | 4.80                 |
| 2649        | <br>$\text{CF}_3\text{CO}_2\text{H}$   | 486.6 (M + H) | 4.64                 |
| 2650        | <br>$\text{CF}_3\text{CO}_2\text{H}$ | 486.6 (M + H) | 4.66                 |



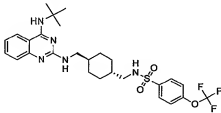
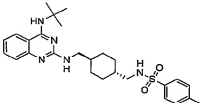
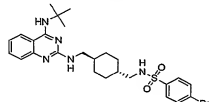
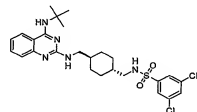
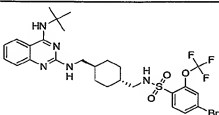
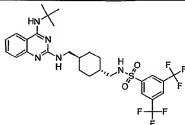
| Example No. | Structure  | ESI-MS        | Retention Time (min) |
|-------------|--|---------------|----------------------|
| 2651        | <br><chem>CC(C)Nc1nc2c(ncn2C1CCCC1NS(=O)(=O)c3ccc(Cl)cc3)nc4ccccc14</chem><br>$\text{CF}_3\text{CO}_2\text{H}$        | 502.6 (M + H) | 4.72                 |
| 2652        | <br><chem>CC(C)Nc1nc2c(ncn2C1CCCC1NS(=O)(=O)c3cccc(Cl)c3)nc4ccccc14</chem><br>$\text{CF}_3\text{CO}_2\text{H}$        | 502.6 (M + H) | 4.87                 |
| 2653        | <br><chem>CC(C)Nc1nc2c(ncn2C1CCCC1NS(=O)(=O)c3cc(F)(F)Fcc(Cl)c3)nc4ccccc14</chem><br>$\text{CF}_3\text{CO}_2\text{H}$ | 570.6 (M + H) | 5.03                 |
| 2654        | <br><chem>CC(C)Nc1nc2c(ncn2C1CCCC1NS(=O)(=O)c3cccc(Br)c3)nc4ccccc14</chem><br>$\text{CF}_3\text{CO}_2\text{H}$        | 546.6 (M + H) | 4.77                 |
| 2655        | <br><chem>CC(C)Nc1nc2c(ncn2C1CCCC1NS(=O)(=O)c3cc(OC)cc(OC)c3)nc4ccccc14</chem><br>$\text{CF}_3\text{CO}_2\text{H}$    | 528.8 (M + H) | 4.68                 |
| 2656        | <br><chem>CC(C)Nc1nc2c(ncn2C1CCCC1NS(=O)(=O)c3cc(F)(F)Fcc3)nc4ccccc14</chem><br>$\text{CF}_3\text{CO}_2\text{H}$    | 552.8 (M + H) | 4.89                 |

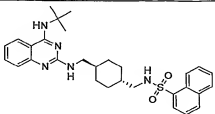
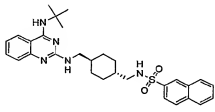
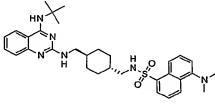
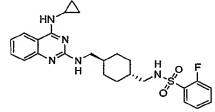
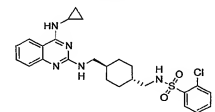
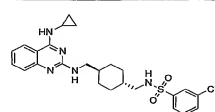
| Example No. | Structure   | ESI-MS        | Retention Time (min) |
|-------------|---|---------------|----------------------|
| 2657        | <br><chem>CC(C)Nc1ncnc2ccccc12C1CCC(CC1)CNS(=O)(=O)c3ccccc3C(F)(F)F</chem><br>$\text{CF}_3\text{CO}_2\text{H}$   | 536.6 (M + H) | 4.85                 |
| 2658        | <br><chem>CC(C)Nc1ncnc2ccccc12C1CCC(CC1)CNS(=O)(=O)c3ccc(C(C)(C)C)cc3</chem><br>$\text{CF}_3\text{CO}_2\text{H}$ | 524.8 (M + H) | 5.15                 |
| 2659        | <br><chem>CC(C)Nc1ncnc2ccccc12C1CCC(CC1)CNS(=O)(=O)c3ccsc3</chem><br>$\text{CF}_3\text{CO}_2\text{H}$            | 474.8 (M + H) | 4.63                 |
| 2660        | <br><chem>CC(C)Nc1ncnc2ccccc12C1CCC(CC1)CNS(=O)(=O)c3ccccc3</chem><br>$\text{CF}_3\text{CO}_2\text{H}$           | 468.4 (M + H) | 4.61                 |
| 2661        | <br><chem>CC(C)Nc1ncnc2ccccc12C1CCC(CC1)CNS(=O)(=O)c3ccc(Cl)cc3</chem><br>$\text{CF}_3\text{CO}_2\text{H}$       | 502.6 (M + H) | 4.86                 |
| 2662        | <br><chem>CC(C)Nc1ncnc2ccccc12C1CCC(CC1)CNS(=O)(=O)c3ccc(Br)cc3</chem><br>$\text{CF}_3\text{CO}_2\text{H}$     | 546.6 (M + H) | 4.64                 |

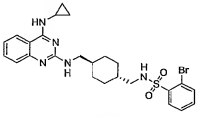
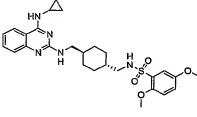
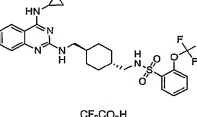
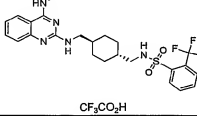
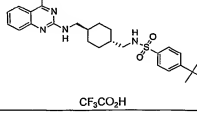
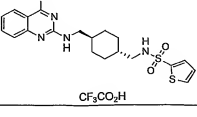
| Example No. | Structure  | ESI-MS        | Retention Time (min) |
|-------------|--|---------------|----------------------|
| 2663        | <br>$\text{CF}_3\text{CO}_2\text{H}$    | 536.4 (M + H) | 4.81                 |
| 2664        | <br>$\text{CF}_3\text{CO}_2\text{H}$    | 630.4 (M + H) | 4.85                 |
| 2665        | <br>$\text{CF}_3\text{CO}_2\text{H}$    | 604.6 (M + H) | 4.87                 |
| 2666        | <br>$\text{CF}_3\text{CO}_2\text{H}$    | 518.6 (M + H) | 4.67                 |
| 2667        | <br>$\text{CF}_3\text{CO}_2\text{H}$   | 518.6 (M + H) | 4.90                 |
| 2668        | <br>$2\text{CF}_3\text{CO}_2\text{H}$ | 561.6 (M + H) | 4.64                 |

| Example No. | Structure  | ESI-MS        | Retention Time (min) |
|-------------|--|---------------|----------------------|
| 2669        |  <p>CF<sub>3</sub>CO<sub>2</sub>H</p>   | 500.8 (M + H) | 4.73                 |
| 2670        |  <p>CF<sub>3</sub>CO<sub>2</sub>H</p>   | 500.8 (M + H) | 4.74                 |
| 2671        |  <p>CF<sub>3</sub>CO<sub>2</sub>H</p>   | 516.6 (M + H) | 4.89                 |
| 2672        |  <p>CF<sub>3</sub>CO<sub>2</sub>H</p>   | 516.6 (M + H) | 4.93                 |
| 2673        |  <p>CF<sub>3</sub>CO<sub>2</sub>H</p>  | 560.0 (M + H) | 4.89                 |
| 2674        |  <p>CF<sub>3</sub>CO<sub>2</sub>H</p> | 542.8 (M + H) | 4.76                 |

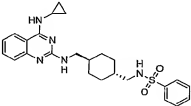
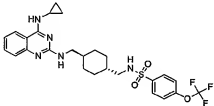
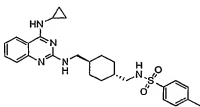
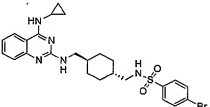
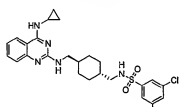
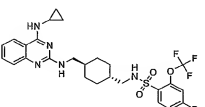


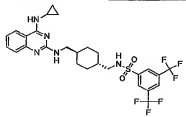
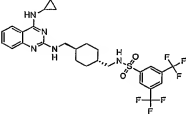
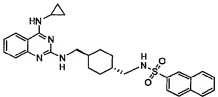
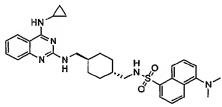
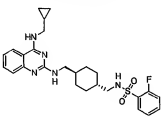
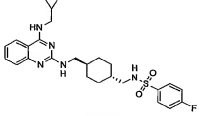
| Example No. | Structure  | ESI-MS        | Retention Time (min) |
|-------------|--|---------------|----------------------|
| 2681        |  <p>CF<sub>3</sub>CO<sub>2</sub>H</p>   | 566.8 (M + H) | 5.07                 |
| 2682        |  <p>CF<sub>3</sub>CO<sub>2</sub>H</p>   | 496.8 (M + H) | 4.83                 |
| 2683        |  <p>CF<sub>3</sub>CO<sub>2</sub>H</p>   | 560.6 (M + H) | 5.01                 |
| 2684        |  <p>CF<sub>3</sub>CO<sub>2</sub>H</p>   | 550.6 (M + H) | 5.07                 |
| 2685        |  <p>CF<sub>3</sub>CO<sub>2</sub>H</p>   | 644.6 (M + H) | 5.29                 |
| 2686        |  <p>CF<sub>3</sub>CO<sub>2</sub>H</p> | 618.6 (M + H) | 5.25                 |

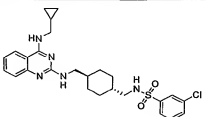
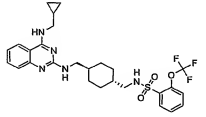
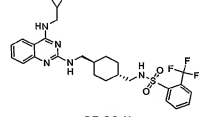
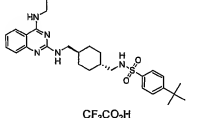
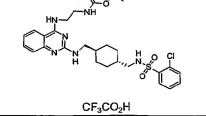
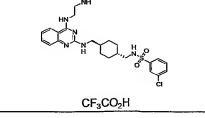
| Example No. | Structure  | ESI-MS        | Retention Time (min) |
|-------------|--|---------------|----------------------|
| 2687        |  <p>CF<sub>3</sub>CO<sub>2</sub>H</p>   | 532.6 (M + H) | 5.01                 |
| 2688        |  <p>CF<sub>3</sub>CO<sub>2</sub>H</p>   | 532.6 (M + H) | 5.04                 |
| 2689        |  <p>2CF<sub>3</sub>CO<sub>2</sub>H</p>  | 575.8 (M + H) | 4.75                 |
| 2690        |  <p>CF<sub>3</sub>CO<sub>2</sub>H</p>   | 484.6 (M + H) | 4.51                 |
| 2691        |  <p>CF<sub>3</sub>CO<sub>2</sub>H</p>   | 500.8 (M + H) | 4.59                 |
| 2692        |  <p>CF<sub>3</sub>CO<sub>2</sub>H</p> | 500.8 (M + H) | 4.71                 |

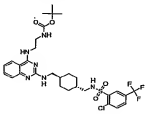
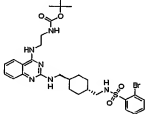
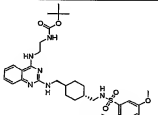
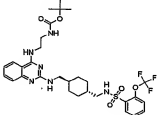
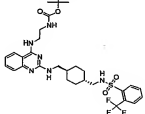
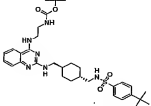
| Example No. | Structure  | ESI-MS        | Retention Time (min) |
|-------------|--|---------------|----------------------|
| 2693        |  <p>CF<sub>3</sub>CO<sub>2</sub>H</p>   | 544.6 (M + H) | 4.63                 |
| 2694        |  <p>CF<sub>3</sub>CO<sub>2</sub>H</p>   | 526.8 (M + H) | 4.55                 |
| 2695        |  <p>CF<sub>3</sub>CO<sub>2</sub>H</p>   | 550.6 (M + H) | 4.79                 |
| 2696        |  <p>CF<sub>3</sub>CO<sub>2</sub>H</p>   | 534.6 (M + H) | 4.69                 |
| 2697        |  <p>CF<sub>3</sub>CO<sub>2</sub>H</p>  | 522.4 (M + H) | 5.03                 |
| 2698        |  <p>CF<sub>3</sub>CO<sub>2</sub>H</p> | 472.8 (M + H) | 4.43                 |

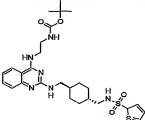
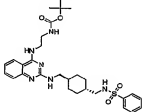
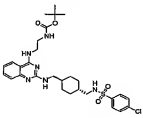
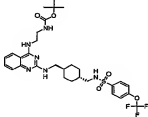
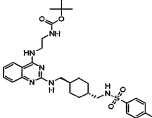
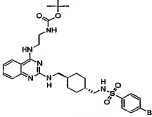


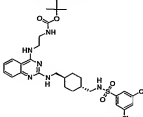
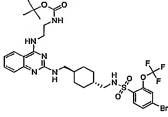
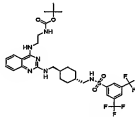
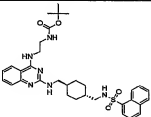
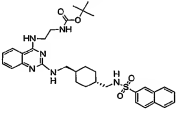
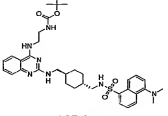
| Example No. | Structure  | ESI-MS        | Retention Time (min) |
|-------------|--|---------------|----------------------|
| 2699        |  <p>CF<sub>3</sub>CO<sub>2</sub>H</p>   | 466.6 (M + H) | 4.50                 |
| 2700        |  <p>CF<sub>3</sub>CO<sub>2</sub>H</p>   | 550.6 (M + H) | 4.87                 |
| 2701        |  <p>CF<sub>3</sub>CO<sub>2</sub>H</p>   | 480.6 (M + H) | 4.65                 |
| 2702        |  <p>CF<sub>3</sub>CO<sub>2</sub>H</p>   | 544.6 (M + H) | 4.75                 |
| 2703        |  <p>CF<sub>3</sub>CO<sub>2</sub>H</p>   | 534.6 (M + H) | 4.90                 |
| 2704        |  <p>CF<sub>3</sub>CO<sub>2</sub>H</p> | 628.6 (M + H) | 5.08                 |

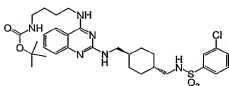
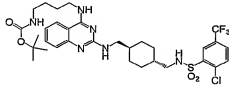
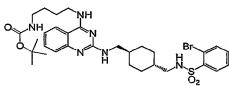
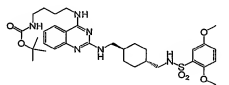
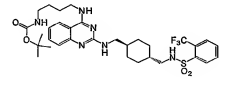
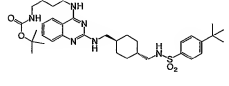
| Example No. | Structure  | ESI-MS        | Retention Time (min) |
|-------------|--|---------------|----------------------|
| 2705        |  <p>CF<sub>3</sub>CO<sub>2</sub>H</p>   | 602.6 (M + H) | 5.10                 |
| 2706        |  <p>CF<sub>3</sub>CO<sub>2</sub>H</p>   | 516.8 (M + H) | 4.71                 |
| 2707        |  <p>CF<sub>3</sub>CO<sub>2</sub>H</p>   | 516.8 (M + H) | 4.81                 |
| 2708        |  <p>2CF<sub>3</sub>CO<sub>2</sub>H</p>  | 559.6 (M + H) | 4.50                 |
| 2709        |  <p>CF<sub>3</sub>CO<sub>2</sub>H</p>   | 498.8 (M + H) | 4.64                 |
| 2710        |  <p>CF<sub>3</sub>CO<sub>2</sub>H</p> | 498.8 (M + H) | 4.73                 |

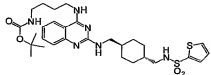
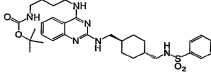
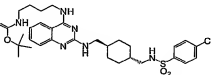
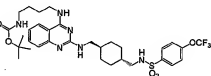
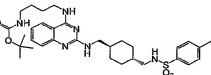
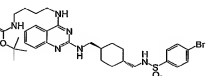
| Example No. | Structure   | ESI-MS        | Retention Time (min) |
|-------------|---|---------------|----------------------|
| 2711        | <br><chem>CC1(C)CC(C1)CNC2=NC3=CC=CC=C3N=C2NS(=O)(=O)c4ccc(Cl)cc4</chem><br>$\text{CF}_3\text{CO}_2\text{H}$               | 514.8 (M + H) | 4.87                 |
| 2712        | <br><chem>CC1(C)CC(C1)CNC2=NC3=CC=CC=C3N=C2NS(=O)(=O)c4cc(F)(F)cc(F)c4</chem><br>$\text{CF}_3\text{CO}_2\text{H}$          | 564.6 (M + H) | 4.93                 |
| 2713        | <br><chem>CC1(C)CC(C1)CNC2=NC3=CC=CC=C3N=C2NS(=O)(=O)c4cc(F)(F)cc(F)c4</chem><br>$\text{CF}_3\text{CO}_2\text{H}$          | 548.6 (M + H) | 4.87                 |
| 2714        | <br><chem>CC1(C)CC(C1)CNC2=NC3=CC=CC=C3N=C2NS(=O)(=O)c4ccc(C(C)(C)C)cc4</chem><br>$\text{CF}_3\text{CO}_2\text{H}$         | 536.6 (M + H) | 5.19                 |
| 2715        | <br><chem>CC(C)(C)OC(=O)NCCNc1nc2ccccc2n(c1)C3=CC=CC=C3NS(=O)(=O)c4ccc(Cl)cc4</chem><br>$\text{CF}_3\text{CO}_2\text{H}$  | 603.8 (M + H) | 4.76                 |
| 2716        | <br><chem>CC(C)(C)OC(=O)NCCNc1nc2ccccc2n(c1)C3=CC=CC=C3NS(=O)(=O)c4ccc(Cl)cc4</chem><br>$\text{CF}_3\text{CO}_2\text{H}$ | 603.4 (M + H) | 4.87                 |

| Example No. | Structure  | ESI-MS        | Retention Time (min) |
|-------------|--|---------------|----------------------|
| 2717        |  <p>CF<sub>3</sub>CO<sub>2</sub>H</p>   | 671.6 (M + H) | 5.05                 |
| 2718        |  <p>CF<sub>3</sub>CO<sub>2</sub>H</p>   | 647.6 (M + H) | 4.79                 |
| 2719        |  <p>CF<sub>3</sub>CO<sub>2</sub>H</p>   | 629.8 (M + H) | 4.67                 |
| 2720        |  <p>CF<sub>3</sub>CO<sub>2</sub>H</p>   | 653.8 (M + H) | 4.91                 |
| 2721        |  <p>CF<sub>3</sub>CO<sub>2</sub>H</p>   | 637.8 (M + H) | 4.85                 |
| 2722        |  <p>CF<sub>3</sub>CO<sub>2</sub>H</p> | 625.8 (M + H) | 5.14                 |

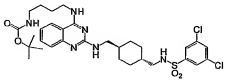
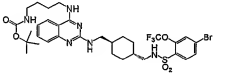
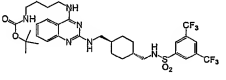
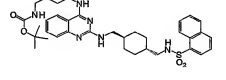
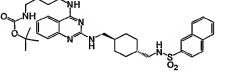
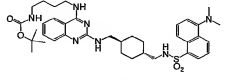
| Example No. | Structure   | ESI-MS        | Retention Time (min) |
|-------------|---|---------------|----------------------|
| 2723        | <br>$\text{CF}_3\text{CO}_2\text{H}$   | 575.6 (M + H) | 4.63                 |
| 2724        | <br>$\text{CF}_3\text{CO}_2\text{H}$   | 569.8 (M + H) | 4.66                 |
| 2725        | <br>$\text{CF}_3\text{CO}_2\text{H}$   | 603.8 (M + H) | 4.88                 |
| 2726        | <br>$\text{CF}_3\text{CO}_2\text{H}$   | 653.8 (M + H) | 5.01                 |
| 2727        | <br>$\text{CF}_3\text{CO}_2\text{H}$   | 583.8 (M + H) | 4.77                 |
| 2728        | <br>$\text{CF}_3\text{CO}_2\text{H}$ | 647 (M + H)   | 4.92                 |

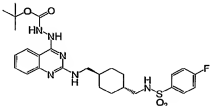
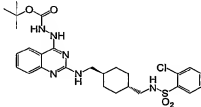
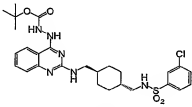
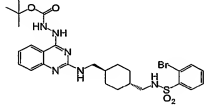
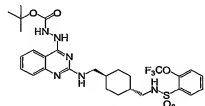
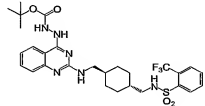
| Example No. | Structure  | ESI-MS        | Retention Time (min) |
|-------------|--|---------------|----------------------|
| 2729        | <br>$\text{CF}_3\text{CO}_2\text{H}$    | 637.8 (M + H) | 5.13                 |
| 2730        | <br>$\text{CF}_3\text{CO}_2\text{H}$    | 731.6 (M + H) | 5.19                 |
| 2731        | <br>$\text{CF}_3\text{CO}_2\text{H}$    | 705.8 (M + H) | 5.22                 |
| 2732        | <br>$\text{CF}_3\text{CO}_2\text{H}$    | 619.8 (M + H) | 4.91                 |
| 2733        | <br>$\text{CF}_3\text{CO}_2\text{H}$    | 619.8 (M + H) | 4.93                 |
| 2734        | <br>$2\text{CF}_3\text{CO}_2\text{H}$ | 663.0 (M + H) | 4.67                 |

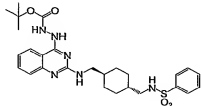
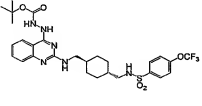
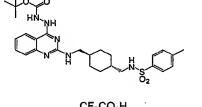
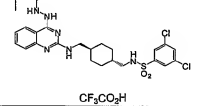
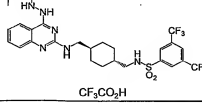
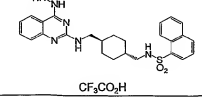
| Example No. | Structure  | ESI-MS        | Retention Time (min) |
|-------------|--|---------------|----------------------|
| 2735        |  <p><math>\text{CF}_3\text{CO}_2\text{H}</math></p>   | 631.8 (M + H) | 5.01                 |
| 2736        |  <p><math>\text{CF}_3\text{CO}_2\text{H}</math></p>   | 699.0 (M + H) | 5.19                 |
| 2737        |  <p><math>\text{CF}_3\text{CO}_2\text{H}</math></p>   | 675.8 (M + H) | 4.95                 |
| 2738        |  <p><math>\text{CF}_3\text{CO}_2\text{H}</math></p>   | 657.8 (M + H) | 4.81                 |
| 2739        |  <p><math>\text{CF}_3\text{CO}_2\text{H}</math></p>   | 665.8 (M + H) | 4.97                 |
| 2740        |  <p><math>\text{CF}_3\text{CO}_2\text{H}</math></p> | 653.8 (M + H) | 5.27                 |

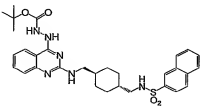
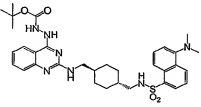
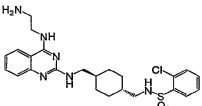
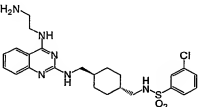
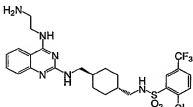
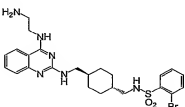
| Example No. | Structure   | ESI-MS        | Retention Time (min) |
|-------------|---|---------------|----------------------|
| 2741        | <br>$\text{CF}_3\text{CO}_2\text{H}$   | 603.4 (M + H) | 4.77                 |
| 2742        | <br>$\text{CF}_3\text{CO}_2\text{H}$   | 597.8 (M + H) | 4.79                 |
| 2743        | <br>$\text{CF}_3\text{CO}_2\text{H}$   | 631.8 (M + H) | 5.02                 |
| 2744        | <br>$\text{CF}_3\text{CO}_2\text{H}$   | 681.8 (M + H) | 5.14                 |
| 2745        | <br>$\text{CF}_3\text{CO}_2\text{H}$   | 611.8 (M + H) | 4.93                 |
| 2746        | <br>$\text{CF}_3\text{CO}_2\text{H}$ | 675.0 (M + H) | 5.05                 |

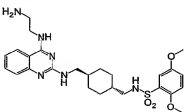
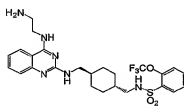
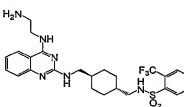
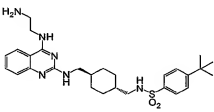
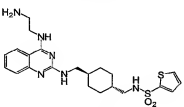
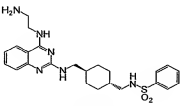


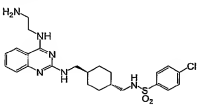
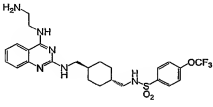
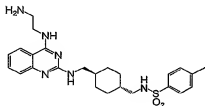
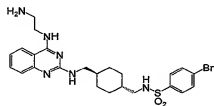
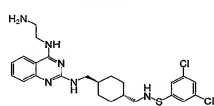
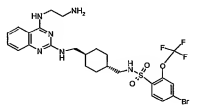
| Example No. | Structure   | ESI-MS        | Retention Time (min) |
|-------------|---|---------------|----------------------|
| 2747        |  <p><math>\text{CF}_3\text{CO}_2\text{H}</math></p>    | 665.8 (M + H) | 5.29                 |
| 2748        |  <p><math>\text{CF}_3\text{CO}_2\text{H}</math></p>    | 759.6 (M + H) | 5.31                 |
| 2749        |  <p><math>\text{CF}_3\text{CO}_2\text{H}</math></p>    | 733.8 (M + H) | 5.36                 |
| 2750        |  <p><math>\text{CF}_3\text{CO}_2\text{H}</math></p>    | 647.8 (M + H) | 5.05                 |
| 2751        |  <p><math>\text{CF}_3\text{CO}_2\text{H}</math></p>    | 647.8 (M + H) | 5.08                 |
| 2752        |  <p><math>2\text{CF}_3\text{CO}_2\text{H}</math></p> | 691.0 (M + H) | 4.89                 |

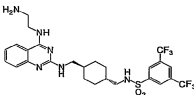
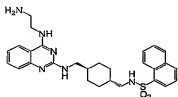
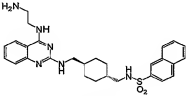
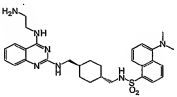
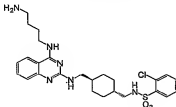
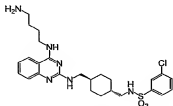
| Example No. | Structure  | ESI-MS        | Retention Time (min) |
|-------------|--|---------------|----------------------|
| 2753        |  <p>CF<sub>3</sub>CO<sub>2</sub>H</p>   | 559.6 (M + H) | 4.51                 |
| 2754        |  <p>CF<sub>3</sub>CO<sub>2</sub>H</p>   | 575.6 (M + H) | 4.57                 |
| 2755        |  <p>CF<sub>3</sub>CO<sub>2</sub>H</p>   | 575.6 (M + H) | 4.69                 |
| 2756        |  <p>CF<sub>3</sub>CO<sub>2</sub>H</p>   | 619.6 (M + H) | 4.63                 |
| 2757        |  <p>CF<sub>3</sub>CO<sub>2</sub>H</p>   | 625.8 (M + H) | 4.72                 |
| 2758        |  <p>CF<sub>3</sub>CO<sub>2</sub>H</p> | 609.8 (M + H) | 4.67                 |

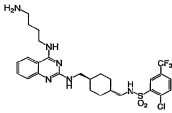
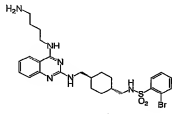
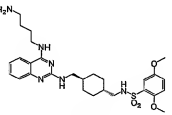
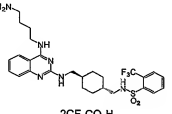
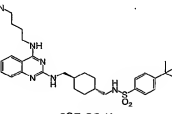
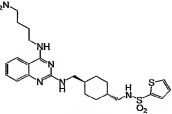
| Example No. | Structure  | ESI-MS        | Retention Time (min) |
|-------------|--|---------------|----------------------|
| 2759        |  <p>CF<sub>3</sub>CO<sub>2</sub>H</p>   | 541.8 (M + H) | 4.45                 |
| 2760        |  <p>CF<sub>3</sub>CO<sub>2</sub>H</p>   | 625.8 (M + H) | 4.38                 |
| 2761        |  <p>CF<sub>3</sub>CO<sub>2</sub>H</p>   | 555.8 (M + H) | 4.57                 |
| 2762        |  <p>CF<sub>3</sub>CO<sub>2</sub>H</p>   | 609.8 (M + H) | 4.94                 |
| 2763        |  <p>CF<sub>3</sub>CO<sub>2</sub>H</p>  | 677.8 (M + H) | 5.05                 |
| 2764        |  <p>CF<sub>3</sub>CO<sub>2</sub>H</p> | 591.6 (M + H) | 4.73                 |

| Example No. | Structure  | ESI-MS        | Retention Time (min) |
|-------------|--|---------------|----------------------|
| 2765        | <br>$\text{CF}_3\text{CO}_2\text{H}$    | 591.6 (M + H) | 4.75                 |
| 2766        | <br>$2\text{CF}_3\text{CO}_2\text{H}$   | 635.0 (M + H) | 4.47                 |
| 2767        | <br>$2\text{CF}_3\text{CO}_2\text{H}$   | 503.6 (M + H) | 3.83                 |
| 2768        | <br>$2\text{CF}_3\text{CO}_2\text{H}$   | 503.6 (M + H) | 3.99                 |
| 2769        | <br>$2\text{CF}_3\text{CO}_2\text{H}$   | 571.6 (M + H) | 4.16                 |
| 2770        | <br>$2\text{CF}_3\text{CO}_2\text{H}$ | 547.6 (M + H) | 3.85                 |

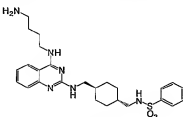
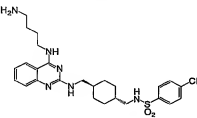
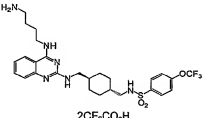
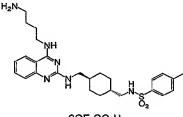
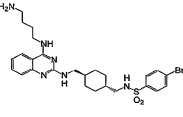
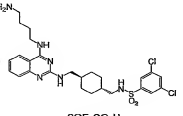
| Example No. | Structure   | ESI-MS        | Retention Time (min) |
|-------------|---|---------------|----------------------|
| 2771        | <br><chem>COc1ccc(cc1)S(=O)(=O)NCCc2ccccc2CNc3nc4ccccc4n3</chem><br>$2CF_3CO_2H$       | 529.6 (M + H) | 3.75                 |
| 2772        | <br><chem>FC(F)(F)c1ccc(cc1)S(=O)(=O)NCCc2ccccc2CNc3nc4ccccc4n3</chem><br>$2CF_3CO_2H$ | 553.8 (M + H) | 3.99                 |
| 2773        | <br><chem>FC(F)(F)c1cccc(c1)S(=O)(=O)NCCc2ccccc2CNc3nc4ccccc4n3</chem><br>$2CF_3CO_2H$ | 537.6 (M + H) | 3.93                 |
| 2774        | <br><chem>CC(C)(C)c1ccc(cc1)S(=O)(=O)NCCc2ccccc2CNc3nc4ccccc4n3</chem><br>$2CF_3CO_2H$ | 525.8 (M + H) | 4.22                 |
| 2775        | <br><chem>c1ccsc1S(=O)(=O)NCCc2ccccc2CNc3nc4ccccc4n3</chem><br>$2CF_3CO_2H$            | 475.6 (M + H) | 3.64                 |
| 2776        | <br><chem>c1ccccc1S(=O)(=O)NCCc2ccccc2CNc3nc4ccccc4n3</chem><br>$2CF_3CO_2H$         | 469.6 (M + H) | 3.71                 |

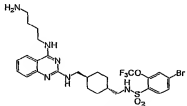
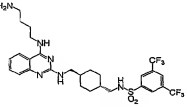
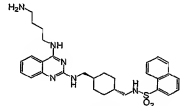
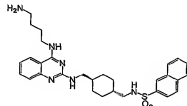
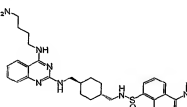
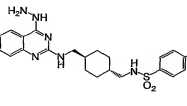
| Example No. | Structure   | ESI-MS        | Retention Time (min) |
|-------------|---|---------------|----------------------|
| 2777        | <br>$2CF_3CO_2H$   | 503.6 (M + H) | 3.97                 |
| 2778        | <br>$2CF_3CO_2H$   | 553.8 (M + H) | 4.17                 |
| 2779        | <br>$2CF_3CO_2H$   | 483.4 (M + H) | 3.87                 |
| 2780        | <br>$2CF_3CO_2H$   | 547.6 (M + H) | 4.04                 |
| 2781        | <br>$2CF_3CO_2H$   | 537.4 (M + H) | 4.23                 |
| 2782        | <br>$2CF_3CO_2H$ | 631.6 (M + H) | 4.23                 |

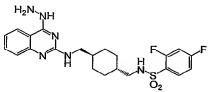
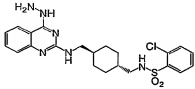
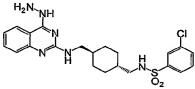
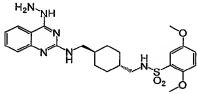
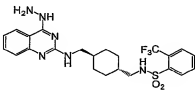
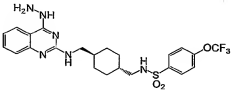
| Example No. | Structure  | ESI-MS        | Retention Time (min) |
|-------------|--|---------------|----------------------|
| 2783        | <br>$2\text{CF}_3\text{CO}_2\text{H}$   | 605.8 (M + H) | 4.41                 |
| 2784        | <br>$2\text{CF}_3\text{CO}_2\text{H}$   | 519.6 (M + H) | 4.01                 |
| 2785        | <br>$2\text{CF}_3\text{CO}_2\text{H}$   | 519.6 (M + H) | 4.07                 |
| 2786        | <br>$3\text{CF}_3\text{CO}_2\text{H}$   | 562.6 (M + H) | 3.77                 |
| 2787        | <br>$2\text{CF}_3\text{CO}_2\text{H}$   | 531.6 (M + H) | 3.90                 |
| 2788        | <br>$2\text{CF}_3\text{CO}_2\text{H}$ | 531.6 (M + H) | 4.04                 |

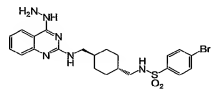
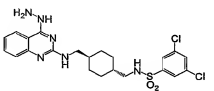
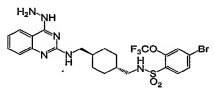
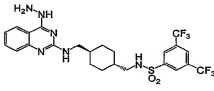
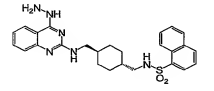
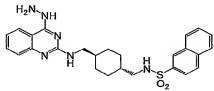
| Example No. | Structure  | ESI-MS        | Retention Time (min) |
|-------------|--|---------------|----------------------|
| 2789        | <br>$2\text{CF}_3\text{CO}_2\text{H}$   | 599.6 (M + H) | 4.24                 |
| 2790        | <br>$2\text{CF}_3\text{CO}_2\text{H}$   | 575.0 (M + H) | 3.95                 |
| 2791        | <br>$2\text{CF}_3\text{CO}_2\text{H}$   | 557.6 (M + H) | 3.86                 |
| 2792        | <br>$2\text{CF}_3\text{CO}_2\text{H}$   | 565.6 (M + H) | 4.03                 |
| 2793        | <br>$2\text{CF}_3\text{CO}_2\text{H}$  | 554 (M + H)   | 4.29                 |
| 2794        | <br>$2\text{CF}_3\text{CO}_2\text{H}$ | 503.6 (M + H) | 3.78                 |



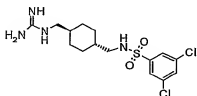
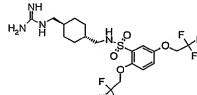
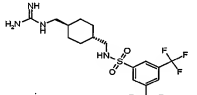
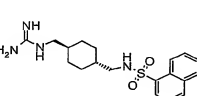
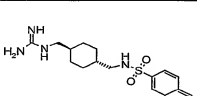
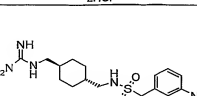
| Example No. | Structure  | ESI-MS        | Retention Time (min) |
|-------------|--|---------------|----------------------|
| 2795        | <br>$2\text{CF}_3\text{CO}_2\text{H}$   | 497.6 (M + H) | 3.83                 |
| 2796        | <br>$2\text{CF}_3\text{CO}_2\text{H}$   | 531.6 (M + H) | 4.05                 |
| 2797        | <br>$2\text{CF}_3\text{CO}_2\text{H}$   | 582.0 (M + H) | 4.23                 |
| 2798        | <br>$2\text{CF}_3\text{CO}_2\text{H}$   | 511 (M + H)   | 3.95                 |
| 2799        | <br>$2\text{CF}_3\text{CO}_2\text{H}$   | 575.6 (M + H) | 4.10                 |
| 2800        | <br>$2\text{CF}_3\text{CO}_2\text{H}$ | 565.0 (M + H) | 4.32                 |

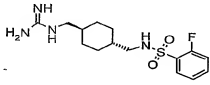
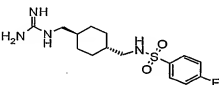
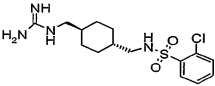
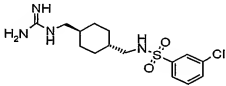
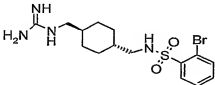
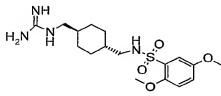
| Example No. | Structure   | ESI-MS        | Retention Time (min) |
|-------------|---|---------------|----------------------|
| 2801        |  <p>2CF<sub>3</sub>CO<sub>2</sub>H</p>   | 659.6 (M + H) | 4.35                 |
| 2802        |  <p>2CF<sub>3</sub>CO<sub>2</sub>H</p>   | 634.0 (M + H) | 4.43                 |
| 2803        |  <p>2CF<sub>3</sub>CO<sub>2</sub>H</p>   | 547.6 (M + H) | 4.09                 |
| 2804        |  <p>2CF<sub>3</sub>CO<sub>2</sub>H</p>   | 547.6 (M + H) | 4.15                 |
| 2805        |  <p>3CF<sub>3</sub>CO<sub>2</sub>H</p>   | 590.6 (M + H) | 3.93                 |
| 2806        |  <p>2CF<sub>3</sub>CO<sub>2</sub>H</p> | 459.6 (M + H) | 4.07                 |

| Example No. | Structure   | ESI-MS        | Retention Time (min) |
|-------------|---|---------------|----------------------|
| 2807        | <br><chem>Nc1nc2ccccc2n1CNC(CCCNS(=O)(=O)c3cc(F)cc(F)c3)C4CCCCC4</chem><br>$2CF_3CO_2H$        | 477.6 (M + H) | 4.07                 |
| 2808        | <br><chem>Nc1nc2ccccc2n1CNC(CCCNS(=O)(=O)c3ccccc3Cl)C4CCCCC4</chem><br>$2CF_3CO_2H$            | 475.6 (M + H) | 4.07                 |
| 2809        | <br><chem>Nc1nc2ccccc2n1CNC(CCCNS(=O)(=O)c3cccc(Cl)c3)C4CCCCC4</chem><br>$2CF_3CO_2H$          | 475.6 (M + H) | 4.23                 |
| 2810        | <br><chem>Nc1nc2ccccc2n1CNC(CCCNS(=O)(=O)c3cc(OC)cc(OC)c3)C4CCCCC4</chem><br>$2CF_3CO_2H$      | 501.8 (M + H) | 4.15                 |
| 2811        | <br><chem>Nc1nc2ccccc2n1CNC(CCCNS(=O)(=O)c3ccccc3C(F)(F)F)C4CCCCC4</chem><br>$2CF_3CO_2H$      | 509.4 (M + H) | 4.27                 |
| 2812        | <br><chem>Nc1nc2ccccc2n1CNC(CCCNS(=O)(=O)c3ccc(OC(F)(F)F)cc3)C4CCCCC4</chem><br>$2CF_3CO_2H$ | 525.6 (M + H) | 4.37                 |

| Example No. | Structure   | ESI-MS        | Retention Time (min) |
|-------------|---|---------------|----------------------|
| 2813        |  <p>2CF<sub>3</sub>CO<sub>2</sub>H</p>   | 519.6 (M + H) | 4.25                 |
| 2814        |  <p>2CF<sub>3</sub>CO<sub>2</sub>H</p>   | 509.4 (M + H) | 4.49                 |
| 2815        |  <p>2CF<sub>3</sub>CO<sub>2</sub>H</p>   | 603.0 (M + H) | 4.60                 |
| 2816        |  <p>2CF<sub>3</sub>CO<sub>2</sub>H</p>   | 577.6 (M + H) | 4.72                 |
| 2817        |  <p>2CF<sub>3</sub>CO<sub>2</sub>H</p>   | 491 (M + H)   | 4.31                 |
| 2818        |  <p>2CF<sub>3</sub>CO<sub>2</sub>H</p> | 491.6 (M + H) | 4.33                 |

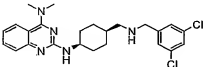
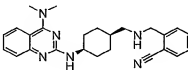
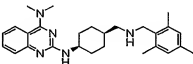
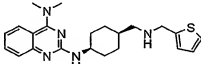
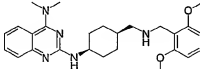
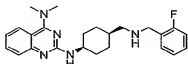


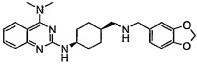
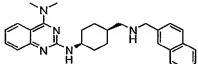
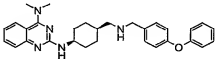
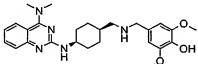
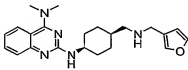
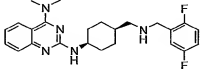
| Example No. | Structure   | ESI-MS        | Retention Time (min) |
|-------------|---|---------------|----------------------|
| 2825        |  <p>2HCl</p>   | 393.0 (M + H) | 4.57                 |
| 2826        |  <p>2HCl</p>   | 521.6 (M + H) | 4.69                 |
| 2827        |  <p>2HCl</p>   | 461.6 (M + H) | 4.77                 |
| 2828        |  <p>2HCl</p>   | 375.4 (M + H) | 4.33                 |
| 2829        |  <p>2HCl</p>   | 375.4 (M + H) | 4.39                 |
| 2830        |  <p>2HCl</p> | 418.8 (M + H) | 4.33                 |

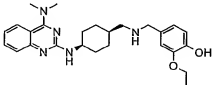
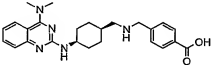
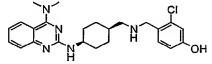
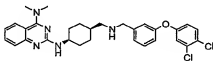
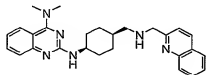
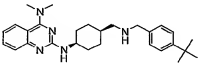
| Example No. | Structure   | ESI-MS        | Retention Time (min) |
|-------------|---|---------------|----------------------|
| 2831        | <br>2HCl   | 343.4 (M + H) | 3.96                 |
| 2832        | <br>2HCl   | 343.4 (M + H) | 4.03                 |
| 2833        | <br>2HCl   | 359.4 (M + H) | 4.05                 |
| 2834        | <br>2HCl   | 359.4 (M + H) | 4.24                 |
| 2835        | <br>2HCl   | 403.4 (M + H) | 4.07                 |
| 2836        | <br>2HCl | 385.4 (M + H) | 4.00                 |

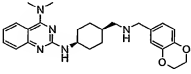
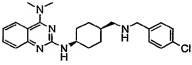
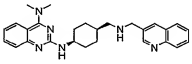
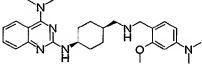
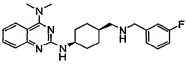
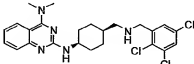
| Example No. | Structure | ESI-MS        | Retention Time (min) |
|-------------|-----------|---------------|----------------------|
| 2837        | <br>2HCl  | 409.4 (M + H) | 4.32                 |
| 2838        | <br>2HCl  | 393.6 (M + H) | 4.23                 |
| 2839        | <br>2HCl  | 381.6 (M + H) | 4.62                 |
| 2840        | <br>2HCl  | 330.8 (M + H) | 3.83                 |
| 2841        | <br>2HCl  | 361.4 (M + H) | 4.05                 |
| 2842        | <br>2HCl  | 427.4 (M + H) | 4.51                 |

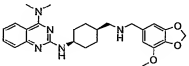
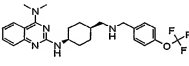
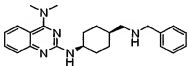
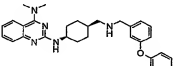
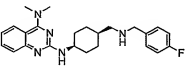
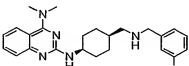


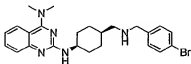
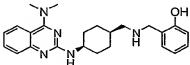
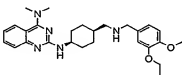
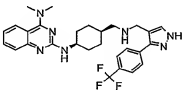
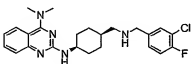
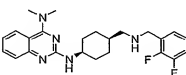
| Example No. | Structure   | ESI-MS        | Retention Time (min) |
|-------------|---|---------------|----------------------|
| 2843        | <br><chem>CC1=NC2=CC=CC=C2N1N[C@H]3CCCC[C@H]3CNCC1=CC=C(C)C=C1Cl</chem><br>$2\text{CF}_3\text{CO}_2\text{H}$           | 458.4 (M + H) | 3.22                 |
| 2844        | <br><chem>CC1=NC2=CC=CC=C2N1N[C@H]3CCCC[C@H]3CNCC1=CC=C(C)C=C1C#N</chem><br>$2\text{CF}_3\text{CO}_2\text{H}$          | 415.4 (M + H) | 3.01                 |
| 2845        | <br><chem>CC1=NC2=CC=CC=C2N1N[C@H]3CCCC[C@H]3CNCC1=CC=C(C)C=C1C</chem><br>$2\text{CF}_3\text{CO}_2\text{H}$            | 432.6 (M + H) | 3.26                 |
| 2846        | <br><chem>CC1=NC2=CC=CC=C2N1N[C@H]3CCCC[C@H]3CNCC1=CC=C(C)C=C1C1=CC=CC=C1S</chem><br>$2\text{CF}_3\text{CO}_2\text{H}$ | 396.2 (M + H) | 2.81                 |
| 2847        | <br><chem>CC1=NC2=CC=CC=C2N1N[C@H]3CCCC[C@H]3CNCC1=CC=C(C)C=C1OC</chem><br>$2\text{CF}_3\text{CO}_2\text{H}$           | 450.0 (M + H) | 3.09                 |
| 2848        | <br><chem>CC1=NC2=CC=CC=C2N1N[C@H]3CCCC[C@H]3CNCC1=CC=C(C)C=C1F</chem><br>$2\text{CF}_3\text{CO}_2\text{H}$          | 408.4 (M + H) | 2.85                 |

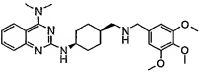
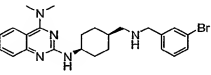
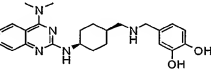
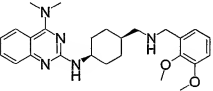
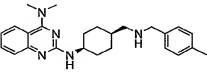
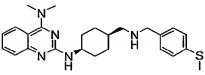
| Example No. | Structure   | ESI-MS        | Retention Time (min) |
|-------------|---|---------------|----------------------|
| 2849        | <br><chem>CC1=C(C)N2C(=N1)N(C)C(=N2)NCC3CCCCC3CCc4ccc5OCOc5c4</chem><br>$2\text{CF}_3\text{CO}_2\text{H}$        | 434.4 (M + H) | 2.89                 |
| 2850        | <br><chem>CC1=C(C)N2C(=N1)N(C)C(=N2)NCC3CCCCC3CCc4ccc(cc4)-c5ccccc5</chem><br>$2\text{CF}_3\text{CO}_2\text{H}$  | 440.0 (M + H) | 3.20                 |
| 2851        | <br><chem>CC1=C(C)N2C(=N1)N(C)C(=N2)NCC3CCCCC3CCc4ccc(cc4)Cc5ccccc5O</chem><br>$2\text{CF}_3\text{CO}_2\text{H}$ | 482.4 (M + H) | 3.43                 |
| 2852        | <br><chem>CC1=C(C)N2C(=N1)N(C)C(=N2)NCC3CCCCC3CCc4ccc(OC)c(OC)c4</chem><br>$2\text{CF}_3\text{CO}_2\text{H}$     | 466.4 (M + H) | 2.71                 |
| 2853        | <br><chem>CC1=C(C)N2C(=N1)N(C)C(=N2)NCC3CCCCC3CCc4ccoc4</chem><br>$2\text{CF}_3\text{CO}_2\text{H}$              | 380.2 (M + H) | 2.72                 |
| 2854        | <br><chem>CC1=C(C)N2C(=N1)N(C)C(=N2)NCC3CCCCC3CCc4cc(F)c(F)cc4</chem><br>$2\text{CF}_3\text{CO}_2\text{H}$     | 426.2 (M + H) | 2.91                 |

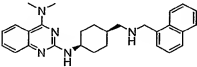
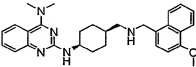
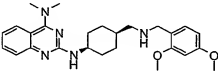
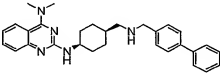
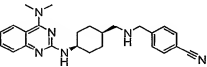
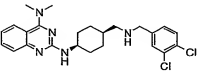
| Example No. | Structure  | ESI-MS        | Retention Time (min) |
|-------------|--|---------------|----------------------|
| 2855        | <br><chem>CCOC1=CC=C(C=C1C(=O)O)CNCCN2CCN(C2)c3ncnc3N4C=NC5=CC=CC=C5N4C5=CC=CC=C5N5C=NC6=CC=CC=C6N5C5=CC=CC=C5N5C=NC6=CC=CC=C6N5</chem><br>$2CF_3CO_2H$ | 450.0 (M + H) | 2.82                 |
| 2856        | <br><chem>OC(=O)C1=CC=C(C=C1)CNCCN2CCN(C2)c3ncnc3N4C=NC5=CC=CC=C5N4C5=CC=CC=C5N5C=NC6=CC=CC=C6N5</chem><br>$2CF_3CO_2H$                                 | 434.4 (M + H) | 2.69                 |
| 2857        | <br><chem>OC1=CC=C(C=C1C(=O)O)C(=O)ClCNCCN2CCN(C2)c3ncnc3N4C=NC5=CC=CC=C5N4C5=CC=CC=C5N5C=NC6=CC=CC=C6N5</chem><br>$2CF_3CO_2H$                         | 440.0 (M + H) | 2.85                 |
| 2858        | <br><chem>ClC1=CC=C(C=C1)OC2=CC=C(C=C2)CNCCN3CCN(C3)c4ncnc4N5C=NC6=CC=CC=C6N5</chem><br>$2CF_3CO_2H$  | 550.6 (M + H) | 3.80                 |
| 2859        | <br><chem>C1=CC=C2C(=C1)N=CN=C2CNCCN3CCN(C3)c4ncnc4N5C=NC6=CC=CC=C6N5</chem><br>$3CF_3CO_2H$  | 441.4 (M + H) | 3.03                 |
| 2860        | <br><chem>CC(C)(C)C1=CC=C(C=C1)CNCCN2CCN(C2)c3ncnc3N4C=NC5=CC=CC=C5N4C5=CC=CC=C5N5C=NC6=CC=CC=C6N5</chem><br>$2CF_3CO_2H$                             | 446.6 (M + H) | 3.41                 |

| Example No. | Structure  | ESI-MS        | Retention Time (min) |
|-------------|--|---------------|----------------------|
| 2861        | <br><chem>CN1C=NC2=CC=CC=C2N1C3CCCCC3NC4=CC=C(C=C4)OC5=CC=CC=C5</chem><br><chem>2CF3CO2H</chem> | 448.4 (M + H) | 2.91                 |
| 2862        | <br><chem>CN1C=NC2=CC=CC=C2N1C3CCCCC3NC4=CC=C(C=C4)Cl</chem><br><chem>2CF3CO2H</chem>           | 424.2 (M + H) | 3.05                 |
| 2863        | <br><chem>CN1C=NC2=CC=CC=C2N1C3CCCCC3NC4=CC=CC=C5N=CC=CC45</chem><br><chem>3CF3CO2H</chem>      | 441.4 (M + H) | 2.68                 |
| 2864        | <br><chem>CN1C=NC2=CC=CC=C2N1C3CCCCC3NC4=CC(=C(C=C4)OC)C</chem><br><chem>3CF3CO2H</chem>        | 463.4 (M + H) | 2.76                 |
| 2865        | <br><chem>CN1C=NC2=CC=CC=C2N1C3CCCCC3NC4=CC=C(C=C4)F</chem><br><chem>2CF3CO2H</chem>            | 408.4 (M + H) | 2.91                 |
| 2866        | <br><chem>CN1C=NC2=CC=CC=C2N1C3CCCCC3NC4=CC(=C(C=C4)Cl)Cl</chem><br><chem>2CF3CO2H</chem>     | 492.2 (M + H) | 3.30                 |

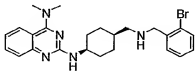
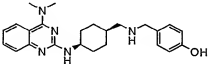
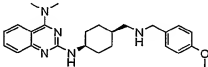
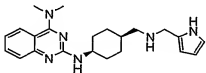
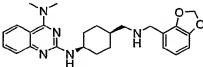
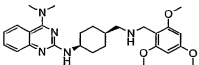
| Example No. | Structure   | ESI-MS        | Retention Time (min) |
|-------------|---|---------------|----------------------|
| 2867        | <br><chem>COc1ccc(cc1)CNCC2(CCC(C)CC2)NCC3=C4C=NC(=C5C=CC=CC=C5N(C)C)N=CN=C43</chem><br>$2\text{CF}_3\text{CO}_2\text{H}$          | 464.2 (M + H) | 2.93                 |
| 2868        | <br><chem>COc1ccc(cc1)CNCC2(CCC(C)CC2)NCC3=C4C=NC(=C5C=CC=CC=C5N(C)C)N=CN=C43</chem><br>$2\text{CF}_3\text{CO}_2\text{H}$          | 474.4 (M + H) | 3.27                 |
| 2869        | <br><chem>c1ccc(cc1)CNCC2(CCC(C)CC2)NCC3=C4C=NC(=C5C=CC=CC=C5N(C)C)N=CN=C43</chem><br>$2\text{CF}_3\text{CO}_2\text{H}$            | 390.6 (M + H) | 2.88                 |
| 2870        | <br><chem>c1ccc(cc1)Oc2ccc(cc2)CNCC3(CCC(C)CC3)NCC4=C5C=NC(=C6C=CC=CC=C6N(C)C)N=CN=C54</chem><br>$2\text{CF}_3\text{CO}_2\text{H}$ | 482.2 (M + H) | 3.43                 |
| 2871        | <br><chem>Fc1ccc(cc1)CNCC2(CCC(C)CC2)NCC3=C4C=NC(=C5C=CC=CC=C5N(C)C)N=CN=C43</chem><br>$2\text{CF}_3\text{CO}_2\text{H}$           | 408.4 (M + H) | 2.91                 |
| 2872        | <br><chem>COc1cccc(c1)CNCC2(CCC(C)CC2)NCC3=C4C=NC(=C5C=CC=CC=C5N(C)C)N=CN=C43</chem><br>$2\text{CF}_3\text{CO}_2\text{H}$        | 420.4 (M + H) | 2.91                 |

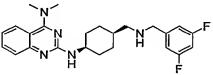
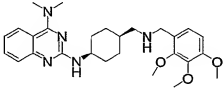
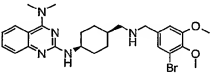
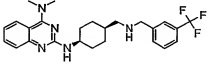
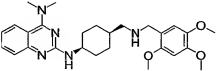
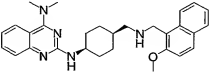
| Example No. | Structure  | ESI-MS        | Retention Time (min) |
|-------------|--|---------------|----------------------|
| 2873        | <br><chem>BrC1=CC=C(C=C1)CNCC2(CCCN2)C3=NC4=CC=CC=C4N(C)C3=NC5=CC=CC=C5N5</chem><br>$2CF_3CO_2H$  | 468.2 (M + H) | 3.09                 |
| 2874        | <br><chem>OC1=CC=C(C=C1)CNCC2(CCCN2)C3=NC4=CC=CC=C4N(C)C3=NC5=CC=CC=C5N5</chem><br>$2CF_3CO_2H$   | 406.4 (M + H) | 2.80                 |
| 2875        | <br><chem>CCOC1=CC=C(C=C1)CNCC2(CCCN2)C3=NC4=CC=CC=C4N(C)C3=NC5=CC=CC=C5N5</chem><br>$2CF_3CO_2H$ | 464.2 (M + H) | 2.97                 |
| 2876        | <br><chem>FC1(F)F=CC=C1CNCC2(CCCN2)C3=NC4=CC=CC=C4N(C)C3=NC5=CC=CC=C5N5</chem><br>$3CF_3CO_2H$    | 524.6 (M + H) | 3.12                 |
| 2877        | <br><chem>Fc1cc(Cl)ccc1CNCC2(CCCN2)C3=NC4=CC=CC=C4N(C)C3=NC5=CC=CC=C5N5</chem><br>$2CF_3CO_2H$    | 442.4 (M + H) | 3.10                 |
| 2878        | <br><chem>Fc1cc(F)ccc1CNCC2(CCCN2)C3=NC4=CC=CC=C4N(C)C3=NC5=CC=CC=C5N5</chem><br>$2CF_3CO_2H$   | 426.2 (M + H) | 2.90                 |

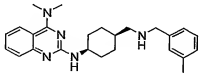
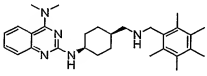
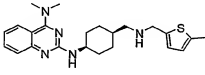
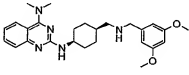
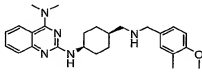
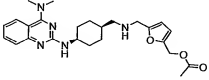
| Example No. | Structure  | ESI-MS        | Retention Time (min) |
|-------------|--|---------------|----------------------|
| 2879        | <br>$2\text{CF}_3\text{CO}_2\text{H}$   | 480.2 (M + H) | 2.89                 |
| 2880        | <br>$2\text{CF}_3\text{CO}_2\text{H}$   | 468.2 (M + H) | 3.07                 |
| 2881        | <br>$2\text{CF}_3\text{CO}_2\text{H}$   | 422.4 (M + H) | 2.61                 |
| 2882        | <br>$2\text{CF}_3\text{CO}_2\text{H}$   | 450.0 (M + H) | 2.93                 |
| 2883        | <br>$2\text{CF}_3\text{CO}_2\text{H}$   | 404.6 (M + H) | 3.01                 |
| 2884        | <br>$2\text{CF}_3\text{CO}_2\text{H}$ | 436.4 (M + H) | 3.08                 |

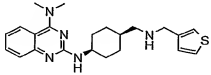
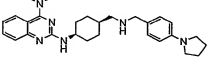
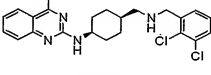
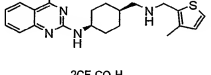
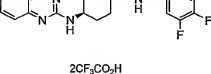
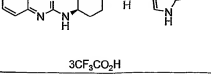
| Example No. | Structure  | ESI-MS        | Retention Time (min) |
|-------------|--|---------------|----------------------|
| 2885        | <br><chem>CN(C)c1nc(NC2CCCCC2Cc3ccccc3)n[nH]1</chem><br>$2CF_3CO_2H$            | 440.0 (M + H) | 3.18                 |
| 2886        | <br><chem>CN(C)c1nc(NC2CCCCC2Cc3ccc(OC)cc3)n[nH]1</chem><br>$2CF_3CO_2H$        | 470.4 (M + H) | 3.25                 |
| 2887        | <br><chem>CN(C)c1nc(NC2CCCCC2Cc3cc(OC)cc(OC)c3)n[nH]1</chem><br>$2CF_3CO_2H$    | 450.0 (M + H) | 3.01                 |
| 2888        | <br><chem>CN(C)c1nc(NC2CCCCC2Cc3ccc(cc3)-c4ccccc4)n[nH]1</chem><br>$2CF_3CO_2H$ | 466.4 (M + H) | 3.40                 |
| 2889        | <br><chem>CN(C)c1nc(NC2CCCCC2Cc3ccc(C#N)cc3)n[nH]1</chem><br>$2CF_3CO_2H$       | 415.4 (M + H) | 2.83                 |
| 2890        | <br><chem>CN(C)c1nc(NC2CCCCC2Cc3cc(Cl)cc(Cl)c3)n[nH]1</chem><br>$2CF_3CO_2H$  | 458.4 (M + H) | 3.25                 |

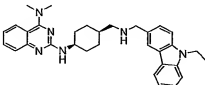
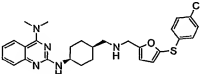
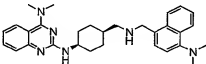
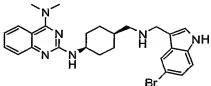
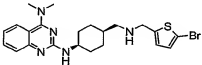
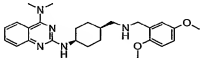


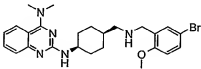
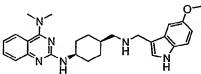
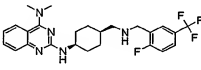
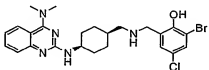
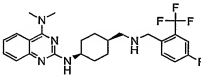
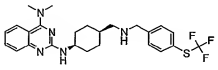
| Example No. | Structure   | ESI-MS        | Retention Time (min) |
|-------------|---|---------------|----------------------|
| 2891        | <br>2CF <sub>3</sub> CO <sub>2</sub> H   | 468.2 (M + H) | 3.00                 |
| 2892        | <br>2CF <sub>3</sub> CO <sub>2</sub> H   | 406.4 (M + H) | 2.66                 |
| 2893        | <br>2CF <sub>3</sub> CO <sub>2</sub> H   | 420.4 (M + H) | 2.92                 |
| 2894        | <br>3CF <sub>3</sub> CO <sub>2</sub> H   | 379.4 (M + H) | 2.71                 |
| 2895        | <br>2CF <sub>3</sub> CO <sub>2</sub> H   | 434.4 (M + H) | 2.87                 |
| 2896        | <br>2CF <sub>3</sub> CO <sub>2</sub> H | 480.2 (M + H) | 3.17                 |

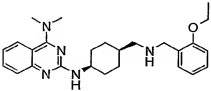
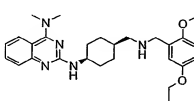
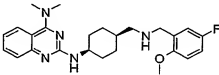
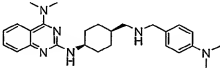
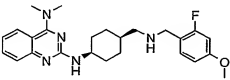
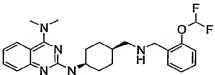
| Example No. | Structure   | ESI-MS        | Retention Time (min) |
|-------------|---|---------------|----------------------|
| 2897        | <br><chem>CN(C)c1nc2ccccc2n1NC3CCCCC3CCNC4=CC=C(C=C4)F</chem><br>$2CF_3CO_2H$            | 426.2 (M + H) | 2.98                 |
| 2898        | <br><chem>CN(C)c1nc2ccccc2n1NC3CCCCC3CCNC4=CC(OC)=C(OC)C=C4OC</chem><br>$2CF_3CO_2H$     | 480.2 (M + H) | 2.99                 |
| 2899        | <br><chem>CN(C)c1nc2ccccc2n1NC3CCCCC3CCNC4=CC(OC)=C(Br)C=C4OC</chem><br>$2CF_3CO_2H$     | 528.4 (M + H) | 3.15                 |
| 2900        | <br><chem>CN(C)c1nc2ccccc2n1NC3CCCCC3CCNC4=CC=C(C=C4)C(F)(F)F</chem><br>$2CF_3CO_2H$     | 458.4 (M + H) | 3.19                 |
| 2901        | <br><chem>CN(C)c1nc2ccccc2n1NC3CCCCC3CCNC4=CC(OC)=C(OC)C=C4OC</chem><br>$2CF_3CO_2H$     | 480.2 (M + H) | 2.92                 |
| 2902        | <br><chem>CN(C)c1nc2ccccc2n1NC3CCCCC3CCNC4=CC5=C(C=C4)C(OC)C=C5</chem><br>$2CF_3CO_2H$ | 470.4 (M + H) | 3.27                 |

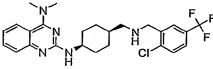
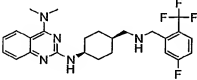
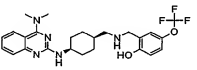
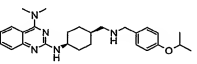
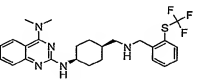
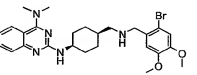
| Example No. | Structure  | ESI-MS        | Retention Time (min) |
|-------------|--|---------------|----------------------|
| 2903        | <br>$2\text{CF}_3\text{CO}_2\text{H}$   | 404.6 (M + H) | 2.87                 |
| 2904        | <br>$2\text{CF}_3\text{CO}_2\text{H}$   | 460.4 (M + H) | 3.48                 |
| 2905        | <br>$2\text{CF}_3\text{CO}_2\text{H}$   | 410.4 (M + H) | 2.96                 |
| 2906        | <br>$2\text{CF}_3\text{CO}_2\text{H}$   | 450.0 (M + H) | 3.03                 |
| 2907        | <br>$2\text{CF}_3\text{CO}_2\text{H}$   | 434.4 (M + H) | 3.08                 |
| 2908        | <br>$2\text{CF}_3\text{CO}_2\text{H}$ | 452.2 (M + H) | 2.79                 |

| Example No. | Structure  | ESI-MS        | Retention Time (min) |
|-------------|--|---------------|----------------------|
| 2909        | <br>$2\text{CF}_3\text{CO}_2\text{H}$   | 396.2 (M + H) | 2.81                 |
| 2910        | <br>$3\text{CF}_3\text{CO}_2\text{H}$   | 459.4 (M + H) | 3.21                 |
| 2911        | <br>$2\text{CF}_3\text{CO}_2\text{H}$   | 458.2 (M + H) | 3.08                 |
| 2912        | <br>$2\text{CF}_3\text{CO}_2\text{H}$   | 410.4 (M + H) | 2.88                 |
| 2913        | <br>$2\text{CF}_3\text{CO}_2\text{H}$  | 426.2 (M + H) | 3.01                 |
| 2914        | <br>$3\text{CF}_3\text{CO}_2\text{H}$ | 429.4 (M + H) | 2.97                 |

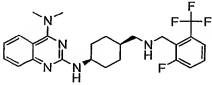
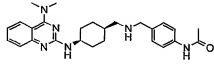
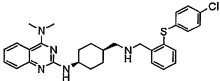
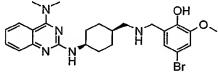
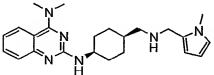
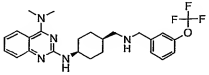
| Example No. | Structure  | ESI-MS        | Retention Time (min) |
|-------------|--|---------------|----------------------|
| 2915        | <br><chem>CC1=CN2C(=N1)N(C)C(=N2)N3CCCCC3N4C(=CC5=CC=CC=C5N(C)C4)CC5</chem><br>$3\text{CF}_3\text{CO}_2\text{H}$            | 507.2 (M + H) | 3.53                 |
| 2916        | <br><chem>CC1=CN2C(=N1)N(C)C(=N2)N3CCCCC3N4C(=CC5=CC=C(C=C5)S4)CC6=CC=C(Cl)C=C6</chem><br>$2\text{CF}_3\text{CO}_2\text{H}$ | 522.4 (M + H) | 3.56                 |
| 2917        | <br><chem>CC1=CN2C(=N1)N(C)C(=N2)N3CCCCC3N4C(=CC5=CC=CC=C5N(C)C4)CC5</chem><br>$3\text{CF}_3\text{CO}_2\text{H}$            | 483.2 (M + H) | 2.80                 |
| 2918        | <br><chem>CC1=CN2C(=N1)N(C)C(=N2)N3CCCCC3N4C(=CC5=CC=CC=C5N(C)C4)CC5</chem><br>$3\text{CF}_3\text{CO}_2\text{H}$            | 507.2 (M + H) | 3.27                 |
| 2919        | <br><chem>CC1=CN2C(=N1)N(C)C(=N2)N3CCCCC3N4C(=CC5=CC=C(C=C5)S4)CC6=CC=C(Br)C=C6</chem><br>$2\text{CF}_3\text{CO}_2\text{H}$ | 474.2 (M + H) | 3.10                 |
| 2920        | <br><chem>CC1=CN2C(=N1)N(C)C(=N2)N3CCCCC3N4C(=CC5=CC(OC)C(OC)C=C5N(C)C4)CC5</chem><br>$2\text{CF}_3\text{CO}_2\text{H}$   | 450.0 (M + H) | 3.00                 |

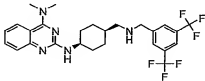
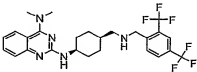
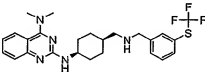
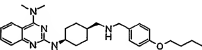
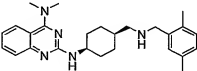
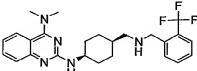
| Example No. | Structure  | ESI-MS        | Retention Time (min) |
|-------------|--|---------------|----------------------|
| 2921        | <br><chem>CN1C=NC2=C(N1)N=CN=C2C3=CC=CC=C3C4=CC=C(C=C4)N5C6CCN(C6)CC5C7=CC=C(C=C7)OC(=O)C8=CC=C(C=C8)Br</chem><br>$2\text{CF}_3\text{CO}_2\text{H}$   | 498.4 (M + H) | 3.15                 |
| 2922        | <br><chem>CN1C=NC2=C(N1)N=CN=C2C3=CC=CC=C3C4=CC=C(C=C4)N5C6CCN(C6)CC5C7=CC=C(C=C7)OC(=O)C8=CC=C(C=C8)Br</chem><br>$3\text{CF}_3\text{CO}_2\text{H}$   | 459.4 (M + H) | 2.99                 |
| 2923        | <br><chem>CN1C=NC2=C(N1)N=CN=C2C3=CC=CC=C3C4=CC=C(C=C4)N5C6CCN(C6)CC5C7=CC=C(C=C7)OC(=O)C8=CC=C(C=C8)Br</chem><br>$2\text{CF}_3\text{CO}_2\text{H}$   | 476.0 (M + H) | 3.10                 |
| 2924        | <br><chem>CN1C=NC2=C(N1)N=CN=C2C3=CC=CC=C3C4=CC=C(C=C4)N5C6CCN(C6)CC5C7=CC=C(C=C7)OC(=O)C8=CC=C(C=C8)Br</chem><br>$2\text{CF}_3\text{CO}_2\text{H}$   | 518.2 (M + H) | 3.10                 |
| 2925        | <br><chem>CN1C=NC2=C(N1)N=CN=C2C3=CC=CC=C3C4=CC=C(C=C4)N5C6CCN(C6)CC5C7=CC=C(C=C7)OC(=O)C8=CC=C(C=C8)Br</chem><br>$2\text{CF}_3\text{CO}_2\text{H}$   | 476.2 (M + H) | 3.12                 |
| 2926        | <br><chem>CN1C=NC2=C(N1)N=CN=C2C3=CC=CC=C3C4=CC=C(C=C4)N5C6CCN(C6)CC5C7=CC=C(C=C7)OC(=O)C8=CC=C(C=C8)Br</chem><br>$2\text{CF}_3\text{CO}_2\text{H}$ | 490.4 (M + H) | 3.35                 |

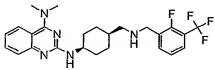
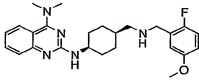
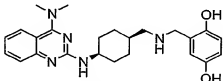
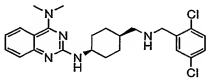
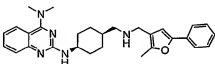
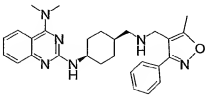
| Example No. | Structure  | ESI-MS        | Retention Time (min) |
|-------------|--|---------------|----------------------|
| 2927        | <br>$2\text{CF}_3\text{CO}_2\text{H}$   | 434.4 (M + H) | 3.11                 |
| 2928        | <br>$2\text{CF}_3\text{CO}_2\text{H}$   | 478.4 (M + H) | 3.29                 |
| 2929        | <br>$2\text{CF}_3\text{CO}_2\text{H}$   | 438.2 (M + H) | 3.01                 |
| 2930        | <br>$3\text{CF}_3\text{CO}_2\text{H}$   | 433.4 (M + H) | 2.59                 |
| 2931        | <br>$2\text{CF}_3\text{CO}_2\text{H}$   | 438.2 (M + H) | 2.90                 |
| 2932        | <br>$2\text{CF}_3\text{CO}_2\text{H}$ | 456.2 (M + H) | 3.10                 |

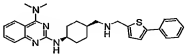
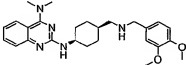
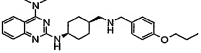
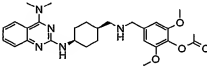
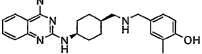
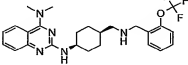
| Example No. | Structure  | ESI-MS        | Retention Time (min) |
|-------------|--|---------------|----------------------|
| 2933        | <br><chem>CN(C)c1nc2c(ncn2C3CCCCC3NC4=CC=C(C(F)(F)F)C=C4Cl)C5=CC=CC=C5</chem><br>$2\text{CF}_3\text{CO}_2\text{H}$                        | 492.2 (M + H) | 3.25                 |
| 2934        | <br><chem>CN(C)c1nc2c(ncn2C3CCCCC3NC4=CC=C(C(F)=C(F)C=C4F)C=C4F)C5=CC=CC=C5</chem><br>$2\text{CF}_3\text{CO}_2\text{H}$                   | 476.2 (M + H) | 3.11                 |
| 2935        | <br><chem>CN(C)c1nc2c(ncn2C3CCCCC3NC4=CC=C(C(=C4)O)OC(F)(F)F)C5=CC=CC=C5</chem><br>$2\text{CF}_3\text{CO}_2\text{H}$                      | 490.4 (M + H) | 3.20                 |
| 2936        | <br><chem>CC(C)Oc1ccc(cc1CNC2CCCCC2NC3=NC4=CC=CC=C4N(C)C3=NC5=CC=CC=C5)N</chem><br>$2\text{CF}_3\text{CO}_2\text{H}$                      | 448.4 (M + H) | 3.17                 |
| 2937        | <br><chem>CN(C)c1nc2c(ncn2C3CCCCC3NC4=CC=C(C(S(=C(F)(F)F)C(F)(F)F)=C4)C=C4)C5=CC=CC=C5</chem><br>$2\text{CF}_3\text{CO}_2\text{H}$        | 489.6 (M + H) | 3.31                 |
| 2938        | <br><chem>COC1=CC=C(C(=C1)C(=C2C=CC(=C2)OC)Br)CNC3CCCCC3NC4=NC5=CC=CC=C5N(C)C4=NC6=CC=CC=C6</chem><br>$2\text{CF}_3\text{CO}_2\text{H}$ | 528.2 (M + H) | 3.03                 |

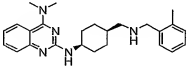
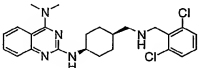
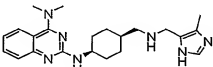
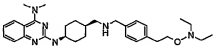
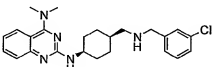
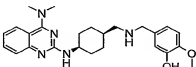


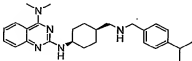
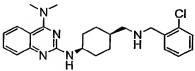
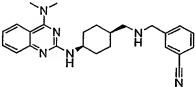
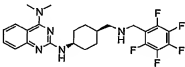
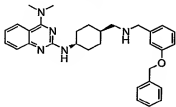
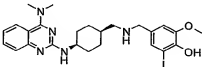
| Example No. | Structure  | ESI-MS        | Retention Time (min) |
|-------------|--|---------------|----------------------|
| 2939        | <br><chem>CC1=NC2=CC=CC=C2N1C3=CC=CC=C3N3C4CCCCC4C5CCN(C5)CC6=CC=C(C=C6)C(F)(F)F</chem><br><chem>CC(F)(F)F(=O)O</chem>        | 476.2 (M + H) | 2.99                 |
| 2940        | <br><chem>CC1=NC2=CC=CC=C2N1C3=CC=CC=C3N3C4CCCCC4C5CCN(C5)CC6=CC=C(C=C6)C(=O)N</chem><br><chem>CC(F)(F)F(=O)O</chem>          | 447.4 (M + H) | 2.66                 |
| 2941        | <br><chem>CC1=NC2=CC=CC=C2N1C3=CC=CC=C3N3C4CCCCC4C5CCN(C5)CC6=CC=C(C=C6)S7=CC=C(C=C7)Cl</chem><br><chem>CC(F)(F)F(=O)O</chem> | 532.4 (M + H) | 3.66                 |
| 2942        | <br><chem>CC1=NC2=CC=CC=C2N1C3=CC=CC=C3N3C4CCCCC4C5CCN(C5)CC6=CC=C(C=C6)C(=O)N</chem><br><chem>CC(F)(F)F(=O)O</chem>          | 514.4 (M + H) | 3.08                 |
| 2943        | <br><chem>CC1=NC2=CC=CC=C2N1C3=CC=CC=C3N3C4CCCCC4C5CCN(C5)CC6=CC=C(C=C6)C(=O)N</chem><br><chem>CC(F)(F)F(=O)O</chem>          | 393.4 (M + H) | 2.79                 |
| 2944        | <br><chem>CC1=NC2=CC=CC=C2N1C3=CC=CC=C3N3C4CCCCC4C5CCN(C5)CC6=CC=C(C=C6)C(=O)N</chem><br><chem>CC(F)(F)F(=O)O</chem>        | 474.4 (M + H) | 3.24                 |

| Example No. | Structure  | ESI-MS        | Retention Time (min) |
|-------------|--|---------------|----------------------|
| 2945        | <br>$2\text{CF}_3\text{CO}_2\text{H}$   | 526.6 (M + H) | 3.44                 |
| 2946        | <br>$2\text{CF}_3\text{CO}_2\text{H}$   | 526.6 (M + H) | 3.42                 |
| 2947        | <br>$2\text{CF}_3\text{CO}_2\text{H}$   | 490.4 (M + H) | 3.35                 |
| 2948        | <br>$2\text{CF}_3\text{CO}_2\text{H}$   | 462.2 (M + H) | 3.43                 |
| 2949        | <br>$2\text{CF}_3\text{CO}_2\text{H}$   | 418.6 (M + H) | 3.13                 |
| 2950        | <br>$2\text{CF}_3\text{CO}_2\text{H}$ | 458.4 (M + H) | 3.10                 |

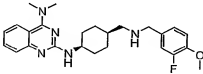
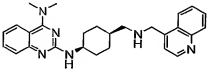
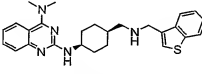
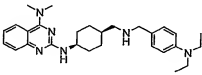
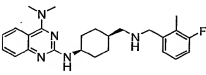
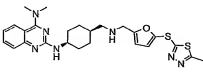
| Example No. | Structure   | ESI-MS        | Retention Time (min) |
|-------------|---|---------------|----------------------|
| 2951        | <br><chem>CC1(C)CCN(C1)C(=O)N(C2=CC=CC=C2N3C(=N(C)N=C3N4C(=CC=C(C=C4)C(F)(F)F)C(F)(F)F)C5=CC=C(C=C5)C(F)(F)F)C6=CC=C(C=C6)C(F)(F)F</chem><br>$2\text{CF}_3\text{CO}_2\text{H}$   | 476.4 (M + H) | 3.19                 |
| 2952        | <br><chem>CC1(C)CCN(C1)C(=O)N(C2=CC=CC=C2N3C(=N(C)N=C3N4C(=CC=C(C=C4)C(F)C)C5=CC=C(C=C5)OC)C6=CC=C(C=C6)OC</chem><br>$2\text{CF}_3\text{CO}_2\text{H}$   | 438.2 (M + H) | 2.95                 |
| 2953        | <br><chem>CC1(C)CCN(C1)C(=O)N(C2=CC=CC=C2N3C(=N(C)N=C3N4C(=CC=C(C=C4)O)C5=CC=C(C=C5)O)C6=CC=C(C=C6)O)C7=CC=C(C=C7)O</chem><br>$2\text{CF}_3\text{CO}_2\text{H}$  | 422.4 (M + H) | 2.61                 |
| 2954        | <br><chem>CC1(C)CCN(C1)C(=O)N(C2=CC=CC=C2N3C(=N(C)N=C3N4C(=CC=C(C=C4)Cl)C5=CC=C(C=C5)Cl)C6=CC=C(C=C6)Cl)C7=CC=C(C=C7)Cl</chem><br>$2\text{CF}_3\text{CO}_2\text{H}$  | 458.2 (M + H) | 3.07                 |
| 2955        | <br><chem>CC1(C)CCN(C1)C(=O)N(C2=CC=CC=C2N3C(=N(C)N=C3N4C(=CC=C(C=C4)C5=CC=C(C=C5)C6=CC=CC=C6O7C(=C(C=C7)C8=CC=CC=C8)C9=CC=CC=C9)C10=CC=C(C=C10)C11=CC=CC=C11)C12=CC=C(C=C12)C13=CC=CC=C13</chem><br>$2\text{CF}_3\text{CO}_2\text{H}$   | 470.4 (M + H) | 3.45                 |
| 2956        | <br><chem>CC1(C)CCN(C1)C(=O)N(C2=CC=CC=C2N3C(=N(C)N=C3N4C(=CC=C(C=C4)C5=CC=C(C=C5)C6=CC=CC=C6O7C(=C(C=C7)C8=CC=CC=C8)C9=CC=CC=C9)C10=CC=C(C=C10)C11=CC=CC=C11)C12=CC=C(C=C12)C13=CC=CC=C13</chem><br>$2\text{CF}_3\text{CO}_2\text{H}$ | 471.6 (M + H) | 2.88                 |

| Example No. | Structure   | ESI-MS        | Retention Time (min) |
|-------------|---|---------------|----------------------|
| 2957        | <br>$2CF_3CO_2H$   | 472.4 (M + H) | 3.36                 |
| 2958        | <br>$2CF_3CO_2H$   | 450 (M + H)   | 2.75                 |
| 2959        | <br>$2CF_3CO_2H$   | 448.4 (M + H) | 3.20                 |
| 2960        | <br>$2CF_3CO_2H$   | 508.4 (M + H) | 3.00                 |
| 2961        | <br>$2CF_3CO_2H$   | 420.4 (M + H) | 2.80                 |
| 2962        | <br>$2CF_3CO_2H$ | 474.4 (M + H) | 3.20                 |

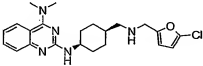
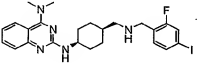
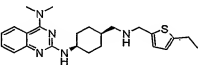
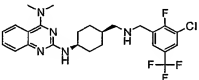
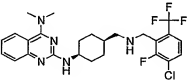
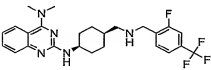
| Example No. | Structure   | ESI-MS        | Retention Time (min) |
|-------------|---|---------------|----------------------|
| 2963        | <br>$2CF_3CO_2H$   | 404.4 (M + H) | 2.87                 |
| 2964        | <br>$2CF_3CO_2H$   | 458.2 (M + H) | 3.00                 |
| 2965        | <br>$3CF_3CO_2H$   | 394.4 (M + H) | 2.30                 |
| 2966        | <br>$2CF_3CO_2H$   | 505.4 (M + H) | 2.60                 |
| 2967        | <br>$2CF_3CO_2H$   | 424.2 (M + H) | 3.00                 |
| 2968        | <br>$2CF_3CO_2H$ | 436.4 (M + H) | 2.71                 |

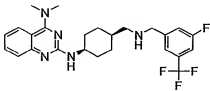
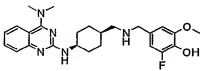
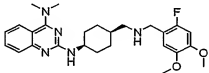
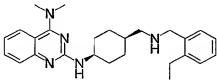
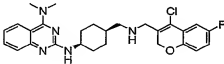
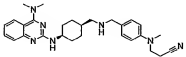
| Example No. | Structure  | ESI-MS        | Retention Time (min) |
|-------------|--|---------------|----------------------|
| 2969        | <br><chem>CC1=CC=C(C=C1)CNCC2CCCCC2Nc3nc(C)c(C)n3</chem><br>$2CF_3CO_2H$            | 432.4 (M + H) | 3.30                 |
| 2970        | <br><chem>Clc1ccc(cc1)CNCC2CCCCC2Nc3nc(C)c(C)n3</chem><br>$2CF_3CO_2H$              | 424.2 (M + H) | 2.95                 |
| 2971        | <br><chem>N#Cc1ccc(cc1)CNCC2CCCCC2Nc3nc(C)c(C)n3</chem><br>$2CF_3CO_2H$             | 415.4 (M + H) | 2.79                 |
| 2972        | <br><chem>Fc1cc(F)c(F)c(F)c1CNCC2CCCCC2Nc3nc(C)c(C)n3</chem><br>$2CF_3CO_2H$        | 480.2 (M + H) | 3.00                 |
| 2973        | <br><chem>c1ccc(cc1)OCC2=CC=C(C=C2)CNCC3CCCCC3Nc4nc(C)c(C)n4</chem><br>$2CF_3CO_2H$ | 496.2 (M + H) | 3.46                 |
| 2974        | <br><chem>COc1cc(I)ccc1CNCC2CCCCC2Nc3nc(C)c(C)n3</chem><br>$2CF_3CO_2H$           | 562.2 (M + H) | 2.99                 |

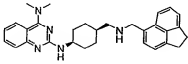
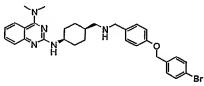
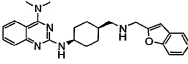
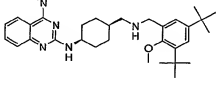
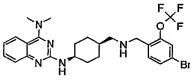
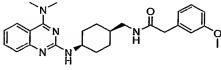


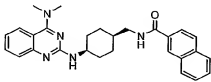
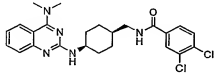
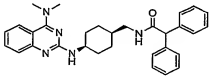
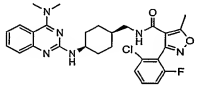
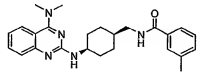
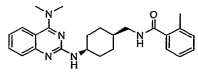
| Example No. | Structure  | ESI-MS        | Retention Time (min) |
|-------------|--|---------------|----------------------|
| 2981        | <br><chem>CC1=NC2=CC=CC=C2N1N(C)C3=CC=C(C=C3)N(C)C3=CC=CC=C3</chem><br>$2CF_3CO_2H$   | 438.2 (M + H) | 2.91                 |
| 2982        | <br><chem>CC1=NC2=CC=CC=C2N1N(C)C3=CC=C(C=C3)N(C)C3=CC=CC=C3</chem><br>$3CF_3CO_2H$   | 441.4 (M + H) | 2.55                 |
| 2983        | <br><chem>CC1=NC2=CC=CC=C2N1N(C)C3=CC=C(C=C3)N(C)C3=CC=CC=C3</chem><br>$2CF_3CO_2H$   | 446.4 (M + H) | 3.13                 |
| 2984        | <br><chem>CC1=NC2=CC=CC=C2N1N(C)C3=CC=C(C=C3)N(C)C3=CC=CC=C3</chem><br>$3CF_3CO_2H$   | 461.4 (M + H) | 2.46                 |
| 2985        | <br><chem>CC1=NC2=CC=CC=C2N1N(C)C3=CC=C(C=C3)N(C)C3=CC=CC=C3</chem><br>$2CF_3CO_2H$   | 422.2 (M + H) | 3.01                 |
| 2986        | <br><chem>CC1=NC2=CC=CC=C2N1N(C)C3=CC=C(C=C3)N(C)C3=CC=CC=C3</chem><br>$2CF_3CO_2H$ | 510.2 (M + H) | 2.85                 |

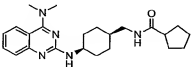
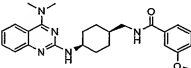
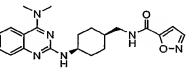
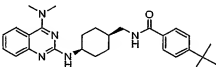
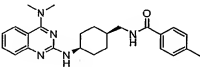
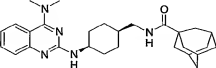


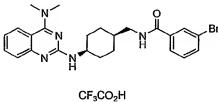
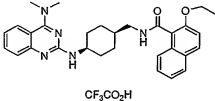
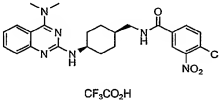
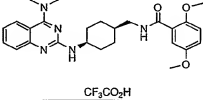
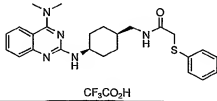
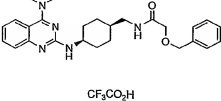
| Example No. | Structure   | ESI-MS        | Retention Time (min) |
|-------------|---|---------------|----------------------|
| 2987        | <br>$2CF_3CO_2H$   | 414.4 (M + H) | 2.86                 |
| 2988        | <br>$2CF_3CO_2H$   | 534.2 (M + H) | 3.13                 |
| 2989        | <br>$2CF_3CO_2H$   | 424.2 (M + H) | 3.08                 |
| 2990        | <br>$2CF_3CO_2H$   | 510.4 (M + H) | 3.32                 |
| 2991        | <br>$2CF_3CO_2H$   | 510.4 (M + H) | 3.17                 |
| 2992        | <br>$2CF_3CO_2H$ | 476.4 (M + H) | 3.17                 |

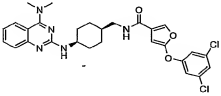
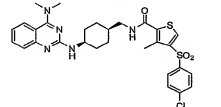
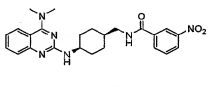
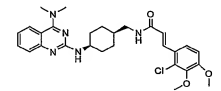
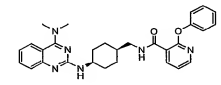
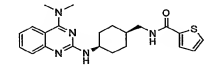
| Example No. | Structure  | ESI-MS        | Retention Time (min) |
|-------------|--|---------------|----------------------|
| 2993        | <br>$2\text{CF}_3\text{CO}_2\text{H}$   | 476.2 (M + H) | 3.21                 |
| 2994        | <br>$2\text{CF}_3\text{CO}_2\text{H}$   | 454.2 (M + H) | 2.77                 |
| 2995        | <br>$2\text{CF}_3\text{CO}_2\text{H}$   | 468.4 (M + H) | 2.89                 |
| 2996        | <br>$2\text{CF}_3\text{CO}_2\text{H}$   | 418.6 (M + H) | 3.12                 |
| 2997        | <br>$2\text{CF}_3\text{CO}_2\text{H}$   | 496.4 (M + H) | 3.29                 |
| 2998        | <br>$3\text{CF}_3\text{CO}_2\text{H}$ | 472.6 (M + H) | 2.99                 |

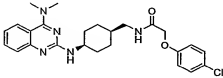
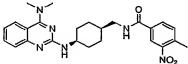
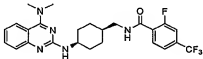
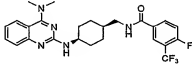
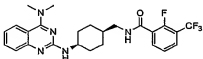
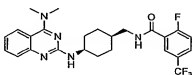
| Example No. | Structure   | ESI-MS        | Retention Time (min) |
|-------------|---|---------------|----------------------|
| 2999        | <br>$2\text{CF}_3\text{CO}_2\text{H}$  | 466.4 (M + H) | 3.37                 |
| 3000        | <br>$2\text{CF}_3\text{CO}_2\text{H}$  | 574.2 (M + H) | 3.64                 |
| 3001        | <br>$2\text{CF}_3\text{CO}_2\text{H}$  | 430.4 (M + H) | 3.05                 |
| 3002        | <br>$2\text{CF}_3\text{CO}_2\text{H}$  | 532.4 (M + H) | 4.05                 |
| 3003        | <br>$2\text{CF}_3\text{CO}_2\text{H}$  | 552.0 (M + H) | 3.37                 |
| 3004        | <br>$\text{CF}_3\text{CO}_2\text{H}$ | 448.4 (M + H) | 3.51                 |

| Example No. | Structure  | ESI-MS        | Retention Time (min) |
|-------------|--|---------------|----------------------|
| 3005        | <br><chem>CC(=O)CCN1CCCC1Nc2nc3ccccc3n2C</chem><br>$\text{CF}_3\text{CO}_2\text{H}$   | 454.2 (M + H) | 3.91                 |
| 3006        | <br><chem>CC(=O)CCN1CCCC1Nc2nc3ccccc3n2Cl</chem><br>$\text{CF}_3\text{CO}_2\text{H}$  | 472.4 (M + H) | 4.02                 |
| 3007        | <br><chem>CC(=O)CCN1CCCC1Nc2nc3ccccc3n2</chem><br>$\text{CF}_3\text{CO}_2\text{H}$    | 494.4 (M + H) | 4.01                 |
| 3008        | <br><chem>CC(=O)CCN1CCCC1Nc2nc3ccccc3n2Cl</chem><br>$\text{CF}_3\text{CO}_2\text{H}$  | 537.4 (M + H) | 3.77                 |
| 3009        | <br><chem>CC(=O)CCN1CCCC1Nc2nc3ccccc3n2C</chem><br>$\text{CF}_3\text{CO}_2\text{H}$   | 418.6 (M + H) | 3.63                 |
| 3010        | <br><chem>CC(=O)CCN1CCCC1Nc2nc3ccccc3n2C</chem><br>$\text{CF}_3\text{CO}_2\text{H}$ | 418.6 (M + H) | 3.51                 |

| Example No. | Structure   | ESI-MS        | Retention Time (min) |
|-------------|---|---------------|----------------------|
| 3011        | <br><chem>CC1=NC2=CC=CC=C2N1N(C)C3=CC=CC=C3N3CCCCC3CNC(=O)C4CCCC4</chem><br>$\text{CF}_3\text{CO}_2\text{H}$                   | 396.2 (M + H) | 3.47                 |
| 3012        | <br><chem>COc1ccc(cc1)C(=O)NCC2CCCCC2N3C=NC4=CC=CC=C4N(C)N3C</chem><br>$\text{CF}_3\text{CO}_2\text{H}$                        | 434.4 (M + H) | 3.52                 |
| 3013        | <br><chem>C1=CC=C(C=C1)O1C=CC(=O)N1CNC2CCCCC2N3C=NC4=CC=CC=C4N(C)N3C</chem><br>$\text{CF}_3\text{CO}_2\text{H}$                | 395.4 (M + H) | 3.15                 |
| 3014        | <br><chem>CC(C)(C)c1ccc(cc1)C(=O)NCC2CCCCC2N3C=NC4=CC=CC=C4N(C)N3C</chem><br>$\text{CF}_3\text{CO}_2\text{H}$                  | 460.2 (M + H) | 4.03                 |
| 3015        | <br><chem>Cc1cccc(c1)C(=O)NCC2CCCCC2N3C=NC4=CC=CC=C4N(C)N3C</chem><br>$\text{CF}_3\text{CO}_2\text{H}$                         | 418.6 (M + H) | 3.65                 |
| 3016        | <br><chem>C1=CC=C(C=C1)N2C=NC3=CC=CC=C3N(C)N2C4CCCCC4CNC(=O)C56C7C=CC8C6C(C7)C5C8</chem><br>$\text{CF}_3\text{CO}_2\text{H}$ | 462.2 (M + H) | 4.09                 |

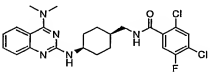
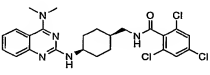
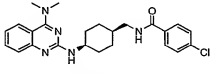
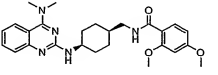
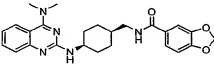
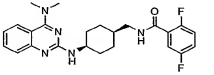
| Example No. | Structure  | ESI-MS        | Retention Time (min) |
|-------------|--|---------------|----------------------|
| 3017        | <br><chem>CN(C)c1nc(NC2CCCCC2CNC(=O)c3ccc(Br)cc3)cnc1C(=O)O.[CF3C(=O)O-]</chem>             | 484.2 (M + H) | 3.79                 |
| 3018        | <br><chem>CN(C)c1nc(NC2CCCCC2CNC(=O)c3ccc(OC)cc3)cnc1C(=O)O.[CF3C(=O)O-]</chem>             | 498.6 (M + H) | 3.88                 |
| 3019        | <br><chem>CN(C)c1nc(NC2CCCCC2CNC(=O)c3cc([N+](=O)[O-])ccc3Cl)cnc1C(=O)O.[CF3C(=O)O-]</chem> | 483.2 (M + H) | 3.80                 |
| 3020        | <br><chem>CN(C)c1nc(NC2CCCCC2CNC(=O)c3ccc(OC)cc3)cnc1C(=O)O.[CF3C(=O)O-]</chem>             | 478.2 (M + H) | 3.49                 |
| 3021        | <br><chem>CN(C)c1nc(NC2CCCCC2CNC(=O)Sc3ccccc3)cnc1C(=O)O.[CF3C(=O)O-]</chem>               | 450.0 (M + H) | 3.61                 |
| 3022        | <br><chem>CN(C)c1nc(NC2CCCCC2CNC(=O)OCc3ccccc3)cnc1C(=O)O.[CF3C(=O)O-]</chem>             | 448.2 (M + H) | 3.70                 |

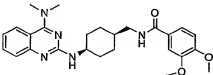
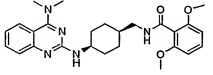
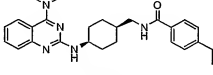
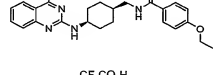
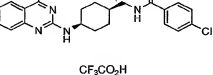
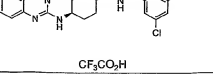
| Example No. | Structure   | ESI-MS        | Retention Time (min) |
|-------------|---|---------------|----------------------|
| 3023        | <br><chem>CC1=NC2=C(N1)N=CN=C2C3=CC=C(C=C3)NCCCCNC(=O)C4=CC(=CC=C4)OC5=CC(=CC=C5)Cl</chem><br>$\text{CF}_3\text{CO}_2\text{H}$         | 554.4 (M + H) | 4.41                 |
| 3024        | <br><chem>CC1=NC2=C(N1)N=CN=C2C3=CC=C(C=C3)NCCCCNC(=O)C4=CC(=CC=C4)S(=O)(=O)C5=CC(=CC=C5)Cl</chem><br>$\text{CF}_3\text{CO}_2\text{H}$ | 598.2 (M + H) | 4.03                 |
| 3025        | <br><chem>CC1=NC2=C(N1)N=CN=C2C3=CC=C(C=C3)NCCCCNC(=O)C4=CC(=CC=C4)[N+](=O)[O-]</chem><br>$\text{CF}_3\text{CO}_2\text{H}$             | 499.2 (M + H) | 3.59                 |
| 3026        | <br><chem>CC1=NC2=C(N1)N=CN=C2C3=CC=C(C=C3)NCCCCNC(=O)C4=CC(=CC=C4)OC5=CC(=CC=C5)Cl</chem><br>$\text{CF}_3\text{CO}_2\text{H}$         | 524.6 (M + H) | 3.84                 |
| 3027        | <br><chem>CC1=NC2=C(N1)N=CN=C2C3=CC=C(C=C3)NCCCCNC(=O)C4=CC=CC=C4N5C=CC=CC=C5</chem><br>$2\text{CF}_3\text{CO}_2\text{H}$              | 497.4 (M + H) | 3.80                 |
| 3028        | <br><chem>CC1=NC2=C(N1)N=CN=C2C3=CC=C(C=C3)NCCCCNC(=O)C4=CC=CC=C4S</chem><br>$\text{CF}_3\text{CO}_2\text{H}$                        | 410.2 (M + H) | 3.43                 |

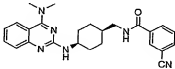
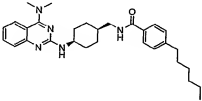
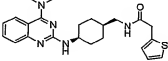
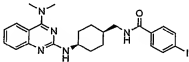
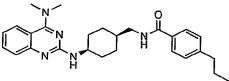
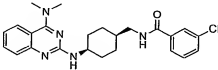
| Example No. | Structure   | ESI-MS        | Retention Time (min) |
|-------------|---|---------------|----------------------|
| 3029        | <br><chem>CC1=NC2=CC=CC=C2N1C(=N)N[C@H]3CCCC[C@H]3CNC(=O)COc4ccc(Cl)cc4</chem><br>$\text{CF}_3\text{CO}_2\text{H}$             | 468.2 (M + H) | 3.77                 |
| 3030        | <br><chem>CC1=NC2=CC=CC=C2N1C(=N)N[C@H]3CCCC[C@H]3CNC(=O)c4cc([N+](=O)[O-])cc(C)c4</chem><br>$\text{CF}_3\text{CO}_2\text{H}$  | 463.2 (M + H) | 3.73                 |
| 3031        | <br><chem>CC1=NC2=CC=CC=C2N1C(=N)N[C@H]3CCCC[C@H]3CNC(=O)c4cc(F)c(C(F)(F)F)c(F)c4</chem><br>$\text{CF}_3\text{CO}_2\text{H}$   | 490.4 (M + H) | 3.91                 |
| 3032        | <br><chem>CC1=NC2=CC=CC=C2N1C(=N)N[C@H]3CCCC[C@H]3CNC(=O)c4cc(F)c(C(F)(F)F)c(F)c4</chem><br>$\text{CF}_3\text{CO}_2\text{H}$   | 490.4 (M + H) | 3.94                 |
| 3033        | <br><chem>CC1=NC2=CC=CC=C2N1C(=N)N[C@H]3CCCC[C@H]3CNC(=O)c4cc(F)c(C(F)(F)F)c(F)c4</chem><br>$\text{CF}_3\text{CO}_2\text{H}$   | 490.4 (M + H) | 3.85                 |
| 3034        | <br><chem>CC1=NC2=CC=CC=C2N1C(=N)N[C@H]3CCCC[C@H]3CNC(=O)c4cc(F)c(C(F)(F)F)c(F)c4</chem><br>$\text{CF}_3\text{CO}_2\text{H}$ | 490.4 (M + H) | 3.87                 |

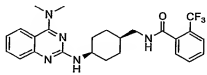
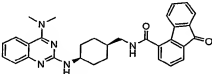
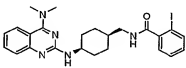
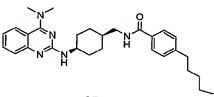
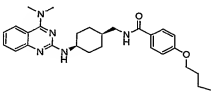
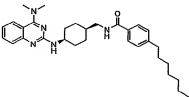


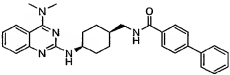
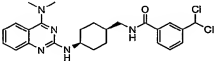
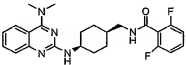
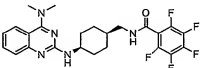
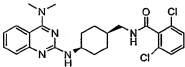
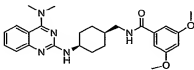


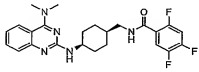
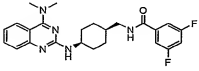
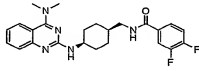
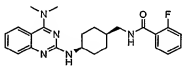
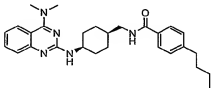
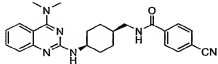
| Example No. | Structure   | ESI-MS        | Retention Time (min) |
|-------------|---|---------------|----------------------|
| 3041        | <br><chem>CC1=C(C)N2C(=N1)N(C)C(=N2)N[C@H]3CCCC[C@H]3CNC(=O)c4cc(Cl)c(F)c(Cl)c4</chem><br>$\text{CF}_3\text{CO}_2\text{H}$ | 490.4 (M + H) | 3.82                 |
| 3042        | <br><chem>CC1=C(C)N2C(=N1)N(C)C(=N2)N[C@H]3CCCC[C@H]3CNC(=O)c4cc(Cl)c(Cl)cc4</chem><br>$\text{CF}_3\text{CO}_2\text{H}$    | 508.0 (M + H) | 3.85                 |
| 3043        | <br><chem>CC1=C(C)N2C(=N1)N(C)C(=N2)N[C@H]3CCCC[C@H]3CNC(=O)c4ccc(Cl)cc4</chem><br>$\text{CF}_3\text{CO}_2\text{H}$        | 438.2 (M + H) | 3.71                 |
| 3044        | <br><chem>CC1=C(C)N2C(=N1)N(C)C(=N2)N[C@H]3CCCC[C@H]3CNC(=O)c4cc(OC)c(OC)cc4</chem><br>$\text{CF}_3\text{CO}_2\text{H}$    | 464.2 (M + H) | 3.65                 |
| 3045        | <br><chem>CC1=C(C)N2C(=N1)N(C)C(=N2)N[C@H]3CCCC[C@H]3CNC(=O)c4c5ccccc5oc4</chem><br>$\text{CF}_3\text{CO}_2\text{H}$       | 448.4 (M + H) | 3.47                 |
| 3046        | <br><chem>CC1=C(C)N2C(=N1)N(C)C(=N2)N[C@H]3CCCC[C@H]3CNC(=O)c4cc(F)c(F)cc4</chem><br>$\text{CF}_3\text{CO}_2\text{H}$    | 440.4 (M + H) | 3.59                 |

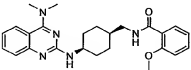
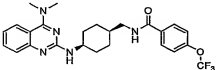
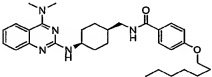
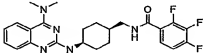
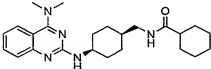
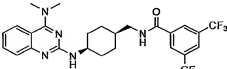
| Example No. | Structure  | ESI-MS        | Retention Time (min) |
|-------------|--|---------------|----------------------|
| 3047        | <br><chem>COc1cc(C(=O)NCC2CCCCC2Nc3nc4ccccc4n3C)cc(OC)c1</chem><br>$\text{CF}_3\text{CO}_2\text{H}$   | 464.2 (M + H) | 3.36                 |
| 3048        | <br><chem>COc1cc(C(=O)NCC2CCCCC2Nc3nc4ccccc4n3C)cc(OC)c1</chem><br>$\text{CF}_3\text{CO}_2\text{H}$   | 464.4 (M + H) | 3.39                 |
| 3049        | <br><chem>CCc1ccc(C(=O)NCC2CCCCC2Nc3nc4ccccc4n3C)cc1</chem><br>$\text{CF}_3\text{CO}_2\text{H}$       | 432.4 (M + H) | 3.81                 |
| 3050        | <br><chem>CCOc1ccc(C(=O)NCC2CCCCC2Nc3nc4ccccc4n3C)cc1</chem><br>$\text{CF}_3\text{CO}_2\text{H}$      | 448.4 (M + H) | 3.69                 |
| 3051        | <br><chem>Clc1ccc(C(=O)NCC2CCCCC2Nc3nc4ccccc4n3C)cc1</chem><br>$\text{CF}_3\text{CO}_2\text{H}$      | 438.2 (M + H) | 3.69                 |
| 3052        | <br><chem>Clc1cc(C(=O)NCC2CCCCC2Nc3nc4ccccc4n3C)cc(Cl)c1</chem><br>$\text{CF}_3\text{CO}_2\text{H}$ | 472.4 (M + H) | 4.03                 |

| Example No. | Structure  | ESI-MS        | Retention Time (min) |
|-------------|--|---------------|----------------------|
| 3053        | <br><chem>CC1=CNC2=CC=CC=C2N1C3CCCCC3CCNC(=O)C4=CC=C(C#N)C=C4</chem><br>$\text{CF}_3\text{CO}_2\text{H}$                      | 429.2 (M + H) | 3.47                 |
| 3054        | <br><chem>CC1=CNC2=CC=CC=C2N1C3CCCCC3CCNC(=O)C4=CC=C(C5=CC=CC=C5C6=CC=CC=C6CC)C=C4</chem><br>$\text{CF}_3\text{CO}_2\text{H}$ | 488.4 (M + H) | 4.60                 |
| 3055        | <br><chem>CC1=CNC2=CC=CC=C2N1C3CCCCC3CCNC(=O)CC4=CC=CC=C4S</chem><br>$\text{CF}_3\text{CO}_2\text{H}$                         | 424.2 (M + H) | 3.41                 |
| 3056        | <br><chem>CC1=CNC2=CC=CC=C2N1C3CCCCC3CCNC(=O)C4=CC=C(I)C=C4</chem><br>$\text{CF}_3\text{CO}_2\text{H}$                        | 530.2 (M + H) | 3.83                 |
| 3057        | <br><chem>CC1=CNC2=CC=CC=C2N1C3CCCCC3CCNC(=O)C4=CC=C(CCC)C=C4</chem><br>$\text{CF}_3\text{CO}_2\text{H}$                      | 446.4 (M + H) | 4.02                 |
| 3058        | <br><chem>CC1=CNC2=CC=CC=C2N1C3CCCCC3CCNC(=O)C4=CC=C(Cl)C=C4</chem><br>$\text{CF}_3\text{CO}_2\text{H}$                     | 438.2 (M + H) | 3.70                 |

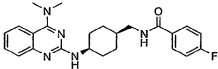
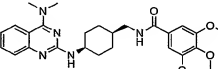
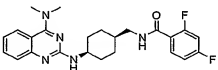
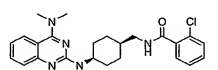
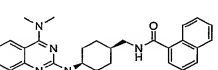
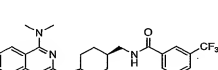
| Example No. | Structure   | ESI-MS        | Retention Time (min) |
|-------------|---|---------------|----------------------|
| 3059        | <br><chem>CC1=C(C2=NC3=CC=CC=C3N(C)N2C4=CC=CC=C4C(=O)O)N(C)C5=CC=CC=C5N(C)C6=CC=CC=C6C(=O)O</chem><br>$\text{CF}_3\text{CO}_2\text{H}$   | 472.4 (M + H) | 3.55                 |
| 3060        | <br><chem>CC1=C(C2=NC3=CC=CC=C3N(C)N2C4=CC=CC=C4C(=O)O)N(C)C5=CC=CC=C5N(C)C6=CC=CC=C6C(=O)O</chem><br>$\text{CF}_3\text{CO}_2\text{H}$   | 506.4 (M + H) | 3.71                 |
| 3061        | <br><chem>CC1=C(C2=NC3=CC=CC=C3N(C)N2C4=CC=CC=C4C(=O)O)N(C)C5=CC=CC=C5N(C)C6=CC=CC=C6C(=O)O</chem><br>$\text{CF}_3\text{CO}_2\text{H}$   | 530.2 (M + H) | 3.61                 |
| 3062        | <br><chem>CC1=C(C2=NC3=CC=CC=C3N(C)N2C4=CC=CC=C4C(=O)O)N(C)C5=CC=CC=C5N(C)C6=CC=CC=C6C(=O)O</chem><br>$\text{CF}_3\text{CO}_2\text{H}$   | 474.4 (M + H) | 4.41                 |
| 3063        | <br><chem>CC1=C(C2=NC3=CC=CC=C3N(C)N2C4=CC=CC=C4C(=O)O)N(C)C5=CC=CC=C5N(C)C6=CC=CC=C6C(=O)O</chem><br>$\text{CF}_3\text{CO}_2\text{H}$   | 476.4 (M + H) | 4.14                 |
| 3064        | <br><chem>CC1=C(C2=NC3=CC=CC=C3N(C)N2C4=CC=CC=C4C(=O)O)N(C)C5=CC=CC=C5N(C)C6=CC=CC=C6C(=O)O</chem><br>$\text{CF}_3\text{CO}_2\text{H}$ | 502.4 (M + H) | 4.83                 |

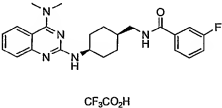
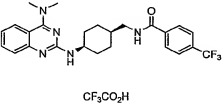
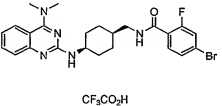
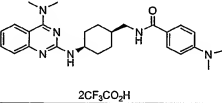
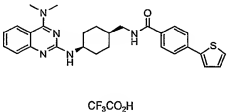
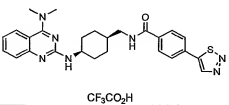
| Example No. | Structure  | ESI-MS        | Retention Time (min) |
|-------------|--|---------------|----------------------|
| 3065        | <br><chem>CC1=NC2=CC=CC=C2N1C3=CC=CC=C3N3C4CCCCC4CC(=O)Nc5ccc(cc5)-c6ccccc6</chem><br>$\text{CF}_3\text{CO}_2\text{H}$  | 480.4 (M + H) | 4.09                 |
| 3066        | <br><chem>CC1=NC2=CC=CC=C2N1C3=CC=CC=C3N3C4CCCCC4CC(=O)Nc5ccc(cc5Cl)Cl</chem><br>$\text{CF}_3\text{CO}_2\text{H}$       | 486.4 (M + H) | 3.84                 |
| 3067        | <br><chem>CC1=NC2=CC=CC=C2N1C3=CC=CC=C3N3C4CCCCC4CC(=O)Nc5cc(F)c(F)cc5</chem><br>$\text{CF}_3\text{CO}_2\text{H}$       | 440.4 (M + H) | 3.46                 |
| 3068        | <br><chem>CC1=NC2=CC=CC=C2N1C3=CC=CC=C3N3C4CCCCC4CC(=O)Nc5c(F)c(F)c(F)c(F)c5</chem><br>$\text{CF}_3\text{CO}_2\text{H}$ | 494.4 (M + H) | 3.79                 |
| 3069        | <br><chem>CC1=NC2=CC=CC=C2N1C3=CC=CC=C3N3C4CCCCC4CC(=O)Nc5cc(Cl)c(Cl)cc5</chem><br>$\text{CF}_3\text{CO}_2\text{H}$     | 472.4 (M + H) | 3.55                 |
| 3070        | <br><chem>CC1=NC2=CC=CC=C2N1C3=CC=CC=C3N3C4CCCCC4CC(=O)Nc5cc(OC)c(OC)cc5</chem><br>$\text{CF}_3\text{CO}_2\text{H}$   | 464.4 (M + H) | 3.63                 |

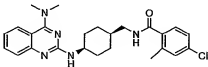
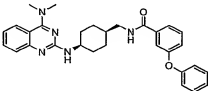
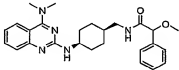
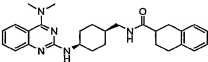
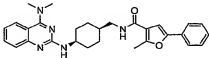
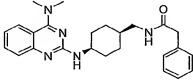
| Example No. | Structure   | ESI-MS        | Retention Time (min) |
|-------------|---|---------------|----------------------|
| 3071        | <br><chem>CC1=NC2=CC=CC=C2N(C)N1C3=CC=C(C=C3)NCC4CCCCC4NC(=O)C5=CC(=CC(=C5)F)F</chem><br>$\text{CF}_3\text{CO}_2\text{H}$  | 458.2 (M + H) | 3.69                 |
| 3072        | <br><chem>CC1=NC2=CC=CC=C2N(C)N1C3=CC=C(C=C3)NCC4CCCCC4NC(=O)C5=CC(=CC(=C5)F)F</chem><br>$\text{CF}_3\text{CO}_2\text{H}$  | 440.4 (M + H) | 3.69                 |
| 3073        | <br><chem>CC1=NC2=CC=CC=C2N(C)N1C3=CC=C(C=C3)NCC4CCCCC4NC(=O)C5=CC(=CC(=C5)F)F</chem><br>$\text{CF}_3\text{CO}_2\text{H}$  | 440.4 (M + H) | 3.66                 |
| 3074        | <br><chem>CC1=NC2=CC=CC=C2N(C)N1C3=CC=C(C=C3)NCC4CCCCC4NC(=O)C5=CC=CC(=C5)F</chem><br>$\text{CF}_3\text{CO}_2\text{H}$     | 422.4 (M + H) | 3.55                 |
| 3075        | <br><chem>CC1=NC2=CC=CC=C2N(C)N1C3=CC=C(C=C3)NCC4CCCCC4NC(=O)C5=CC=C(C=C5)CCC</chem><br>$\text{CF}_3\text{CO}_2\text{H}$   | 460.4 (M + H) | 4.24                 |
| 3076        | <br><chem>CC1=NC2=CC=CC=C2N(C)N1C3=CC=C(C=C3)NCC4CCCCC4NC(=O)C5=CC=C(C=C5)C#N</chem><br>$\text{CF}_3\text{CO}_2\text{H}$ | 429.2 (M + H) | 3.42                 |

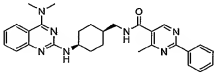
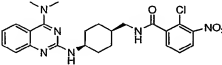
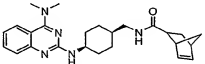
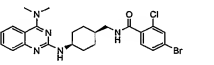
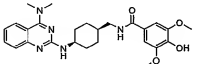
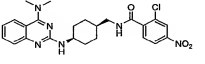
| Example No. | Structure  | ESI-MS        | Retention Time (min) |
|-------------|--|---------------|----------------------|
| 3077        | <br><chem>COc1ccc(cc1)C(=O)NCC2CCCCC2CNc3nc4ccccc4n(C)c3</chem><br>$\text{CF}_3\text{CO}_2\text{H}$               | 434.4 (M + H) | 3.61                 |
| 3078        | <br><chem>COc1ccc(cc1)C(=O)NCC2CCCCC2CNc3nc4ccccc4n(C)c3</chem><br>$\text{CF}_3\text{CO}_2\text{H}$               | 488.4 (M + H) | 3.86                 |
| 3079        | <br><chem>CCOCCc1ccc(cc1)C(=O)NCC2CCCCC2CNc3nc4ccccc4n(C)c3</chem><br>$\text{CF}_3\text{CO}_2\text{H}$            | 518.6 (M + H) | 4.74                 |
| 3080        | <br><chem>Fc1cc(F)ccc1C(=O)NCC2CCCCC2CNc3nc4ccccc4n(C)c3</chem><br>$\text{CF}_3\text{CO}_2\text{H}$               | 458.2 (M + H) | 3.68                 |
| 3081        | <br><chem>C1CCCCC1C(=O)NCC2CCCCC2CNc3nc4ccccc4n(C)c3</chem><br>$\text{CF}_3\text{CO}_2\text{H}$                   | 410.4 (M + H) | 3.58                 |
| 3082        | <br><chem>CC1=CC(=CC(=C1)C(F)(F)F)C(=O)NCC2CCCCC2CNc3nc4ccccc4n(C)c3</chem><br>$\text{CF}_3\text{CO}_2\text{H}$ | 540.4 (M + H) | 4.19                 |

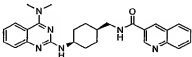
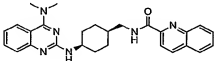
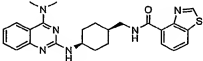
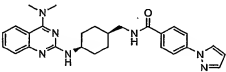
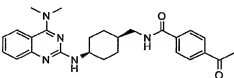
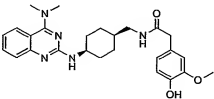


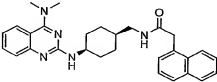
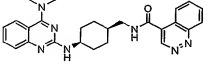
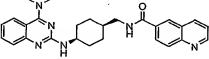
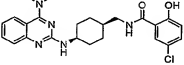
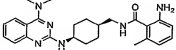
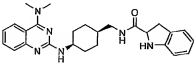
| Example No. | Structure  | ESI-MS        | Retention Time (min) |
|-------------|--|---------------|----------------------|
| 3083        | <br><chem>CCN(C)C1=CC=C(C=C1)N2C(=NC3=CC=CC=C3N2C4=CC=CC=C4)N5CCCCC5CNC(=O)C6=CC=C(C=C6)F</chem><br>$\text{CF}_3\text{CO}_2\text{H}$          | 422.2 (M + H) | 3.50                 |
| 3084        | <br><chem>CCN(C)C1=CC=C(C=C1)N2C(=NC3=CC=CC=C3N2C4=CC=CC=C4)N5CCCCC5CNC(=O)C6=CC(OC)=C(OC)C(OC)=C6</chem><br>$\text{CF}_3\text{CO}_2\text{H}$ | 494.4 (M + H) | 3.39                 |
| 3085        | <br><chem>CCN(C)C1=CC=C(C=C1)N2C(=NC3=CC=CC=C3N2C4=CC=CC=C4)N5CCCCC5CNC(=O)C6=CC(F)=CC(F)=C6</chem><br>$\text{CF}_3\text{CO}_2\text{H}$       | 440.0 (M + H) | 3.55                 |
| 3086        | <br><chem>CCN(C)C1=CC=C(C=C1)N2C(=NC3=CC=CC=C3N2C4=CC=CC=C4)N5CCCCC5CNC(=O)C6=CC(Cl)=CC=C6</chem><br>$\text{CF}_3\text{CO}_2\text{H}$         | 438.2 (M + H) | 3.48                 |
| 3087        | <br><chem>CCN(C)C1=CC=C(C=C1)N2C(=NC3=CC=CC=C3N2C4=CC=CC=C4)N5CCCCC5CNC(=O)C6=CC=CC=C7C=CC=CC67</chem><br>$\text{CF}_3\text{CO}_2\text{H}$    | 454.2 (M + H) | 3.75                 |
| 3088        | <br><chem>CCN(C)C1=CC=C(C=C1)N2C(=NC3=CC=CC=C3N2C4=CC=CC=C4)N5CCCCC5CNC(=O)C6=CC(C(F)(F)F)=CC=C6</chem><br>$\text{CF}_3\text{CO}_2\text{H}$ | 472.4 (M + H) | 3.83                 |

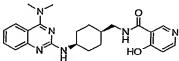
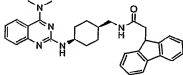
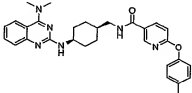
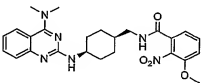
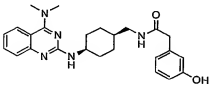
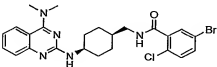
| Example No. | Structure   | ESI-MS        | Retention Time (min) |
|-------------|---|---------------|----------------------|
| 3089        | <br><chem>CC1=NC2=CC=CC=C2N1NCC3CCCCC3NC(=O)c4ccc(F)cc4</chem><br>$\text{CF}_3\text{CO}_2\text{H}$           | 422.2 (M + H) | 3.51                 |
| 3090        | <br><chem>CC1=NC2=CC=CC=C2N1NCC3CCCCC3NC(=O)c4ccc(C(F)(F)F)cc4</chem><br>$\text{CF}_3\text{CO}_2\text{H}$    | 472.4 (M + H) | 3.87                 |
| 3091        | <br><chem>CC1=NC2=CC=CC=C2N1NCC3CCCCC3NC(=O)c4cc(F)cc(Br)c4</chem><br>$\text{CF}_3\text{CO}_2\text{H}$       | 500.4 (M + H) | 3.03                 |
| 3092        | <br><chem>CC1=NC2=CC=CC=C2N1NCC3CCCCC3NC(=O)c4ccc(CN(C)C)cc4</chem><br>$2\text{CF}_3\text{CO}_2\text{H}$     | 447.4 (M + H) | 2.59                 |
| 3093        | <br><chem>CC1=NC2=CC=CC=C2N1NCC3CCCCC3NC(=O)c4ccc(c5ccsc5)cc4</chem><br>$\text{CF}_3\text{CO}_2\text{H}$    | 486.4 (M + H) | 3.25                 |
| 3094        | <br><chem>CC1=NC2=CC=CC=C2N1NCC3CCCCC3NC(=O)c4ccc(c5nn[nH]5)cc4</chem><br>$\text{CF}_3\text{CO}_2\text{H}$ | 488.4 (M + H) | 2.81                 |

| Example No. | Structure  | ESI-MS        | Retention Time (min) |
|-------------|--|---------------|----------------------|
| 3095        | <br><chem>CC1=CC=C(C=C1C(=O)NCC2CCCCC2Nc3ncnc4c3ncn4C)C</chem><br>$\text{CF}_3\text{CO}_2\text{H}$          | 452.4 (M + H) | 2.98                 |
| 3096        | <br><chem>c1ccc(cc1)Oc2ccc(cc2)C(=O)NCC3CCCCC3Nc4ncnc5c4ncn5C</chem><br>$\text{CF}_3\text{CO}_2\text{H}$    | 496.4 (M + H) | 3.29                 |
| 3097        | <br><chem>COC(=O)c1ccccc1C(=O)NCC2CCCCC2Nc3ncnc4c3ncn4C</chem><br>$\text{CF}_3\text{CO}_2\text{H}$          | 448.4 (M + H) | 2.77                 |
| 3098        | <br><chem>C1CCC2C(C1)C(=O)NCC3CCCCC3Nc4ncnc5c4ncn5C</chem><br>$\text{CF}_3\text{CO}_2\text{H}$              | 458.4 (M + H) | 3.06                 |
| 3099        | <br><chem>c1ccccc1c2oc(=O)c(=O)nc2C(=O)NCC3CCCCC3Nc4ncnc5c4ncn5C</chem><br>$\text{CF}_3\text{CO}_2\text{H}$ | 484.4 (M + H) | 3.40                 |
| 3100        | <br><chem>c1ccccc1CC(=O)NCC2CCCCC2Nc3ncnc4c3ncn4C</chem><br>$\text{CF}_3\text{CO}_2\text{H}$              | 418.6 (M + H) | 2.69                 |

| Example No. | Structure   | ESI-MS        | Retention Time (min) |
|-------------|---|---------------|----------------------|
| 3101        | <br>$2\text{CF}_3\text{CO}_2\text{H}$  | 496.4 (M + H) | 3.01                 |
| 3102        | <br>$\text{CF}_3\text{CO}_2\text{H}$   | 483.4 (M + H) | 2.79                 |
| 3103        | <br>$\text{CF}_3\text{CO}_2\text{H}$   | 420.4 (M + H) | 2.76                 |
| 3104        | <br>$\text{CF}_3\text{CO}_2\text{H}$   | 516.2 (M + H) | 3.03                 |
| 3105        | <br>$\text{CF}_3\text{CO}_2\text{H}$   | 480.4 (M + H) | 2.41                 |
| 3106        | <br>$\text{CF}_3\text{CO}_2\text{H}$ | 483.2 (M + H) | 2.84                 |

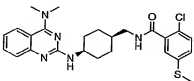
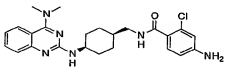
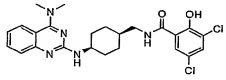
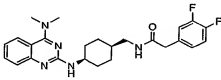
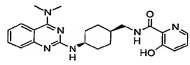
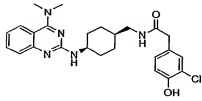
| Example No. | Structure   | ESI-MS        | Retention Time (min) |
|-------------|---|---------------|----------------------|
| 3107        | <br>$2\text{CF}_3\text{CO}_2\text{H}$  | 455 (M + H)   | 2.45                 |
| 3108        | <br>$2\text{CF}_3\text{CO}_2\text{H}$  | 455.2 (M + H) | 3.19                 |
| 3109        | <br>$\text{CF}_3\text{CO}_2\text{H}$   | 461.4 (M + H) | 2.60                 |
| 3110        | <br>$2\text{CF}_3\text{CO}_2\text{H}$  | 470.4 (M + H) | 2.74                 |
| 3111        | <br>$\text{CF}_3\text{CO}_2\text{H}$   | 446.6 (M + H) | 2.61                 |
| 3112        | <br>$\text{CF}_3\text{CO}_2\text{H}$ | 464.4 (M + H) | 2.35                 |

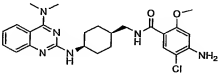
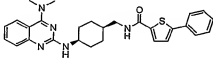
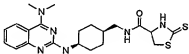
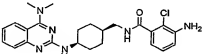
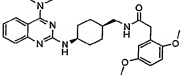
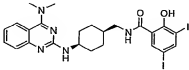
| Example No. | Structure  | ESI-MS        | Retention Time (min) |
|-------------|--|---------------|----------------------|
| 3113        | <br><chem>CC1=NC2=CC=CC=C2N=C(NC3CCCCC3CCNC(=O)Cc4ccc5ccccc45)N1C</chem><br>$\text{CF}_3\text{CO}_2\text{H}$      | 468.4 (M + H) | 3.04                 |
| 3114        | <br><chem>CC1=NC2=CC=CC=C2N=C(NC3CCCCC3CCNC(=O)c4ccncc4)N1C</chem><br>$2\text{CF}_3\text{CO}_2\text{H}$           | 456.2 (M + H) | 2.44                 |
| 3115        | <br><chem>CC1=NC2=CC=CC=C2N=C(NC3CCCCC3CCNC(=O)c4ccc5ncncc45)N1C</chem><br>$2\text{CF}_3\text{CO}_2\text{H}$      | 455.2 (M + H) | 2.11                 |
| 3116        | <br><chem>CC1=NC2=CC=CC=C2N=C(NC3CCCCC3CCNC(=O)c4cc(O)cc(Cl)c4)N1C</chem><br>$\text{CF}_3\text{CO}_2\text{H}$     | 454.2 (M + H) | 3.21                 |
| 3117        | <br><chem>CC1=NC2=CC=CC=C2N=C(NC3CCCCC3CCNC(=O)c4cc(C)c(N)cc4)N1C</chem><br>$2\text{CF}_3\text{CO}_2\text{H}$     | 433.6 (M + H) | 2.34                 |
| 3118        | <br><chem>CC1=NC2=CC=CC=C2N=C(NC3CCCCC3CCNC(=O)c4c[nH]c5ccccc45)N1C</chem><br>$2\text{CF}_3\text{CO}_2\text{H}$ | 444.6 (M+)    | 2.93                 |

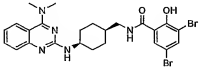
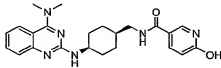
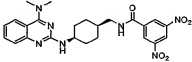
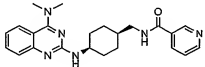
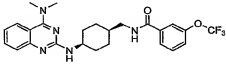
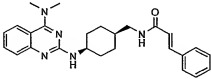
| Example No. | Structure   | ESI-MS        | Retention Time (min) |
|-------------|---|---------------|----------------------|
| 3119        | <br>$2\text{CF}_3\text{CO}_2\text{H}$  | 421.4 (M + H) | 2.23                 |
| 3120        | <br>$\text{CF}_3\text{CO}_2\text{H}$   | 506.4 (M + H) | 3.31                 |
| 3121        | <br>$2\text{CF}_3\text{CO}_2\text{H}$  | 511.6 (M + H) | 3.21                 |
| 3122        | <br>$\text{CF}_3\text{CO}_2\text{H}$   | 479.4 (M + H) | 3.60                 |
| 3123        | <br>$\text{CF}_3\text{CO}_2\text{H}$   | 434.4 (M + H) | 2.37                 |
| 3124        | <br>$\text{CF}_3\text{CO}_2\text{H}$ | 516.4 (M + H) | 3.02                 |

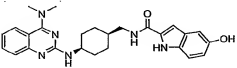
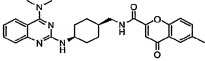
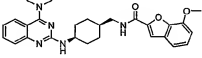
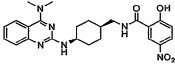
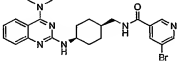
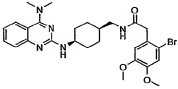




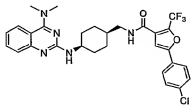
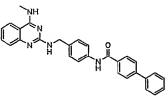
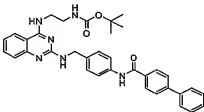
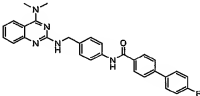
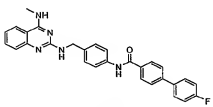
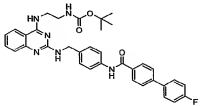
| Example No. | Structure  | ESI-MS        | Retention Time (min) |
|-------------|--|---------------|----------------------|
| 3131        |  <p>CF<sub>3</sub>CO<sub>2</sub>H</p>   | 484.2 (M + H) | 2.99                 |
| 3132        |  <p>2CF<sub>3</sub>CO<sub>2</sub>H</p>  | 453.0 (M + H) | 2.45                 |
| 3133        |  <p>CF<sub>3</sub>CO<sub>2</sub>H</p>   | 488.4 (M + H) | 3.59                 |
| 3134        |  <p>CF<sub>3</sub>CO<sub>2</sub>H</p>   | 454.2 (M + H) | 2.81                 |
| 3135        |  <p>2CF<sub>3</sub>CO<sub>2</sub>H</p>  | 421.4 (M + H) | 2.89                 |
| 3136        |  <p>CF<sub>3</sub>CO<sub>2</sub>H</p> | 468.4 (M + H) | 2.53                 |

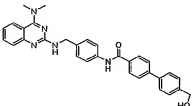
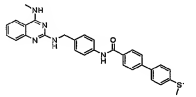
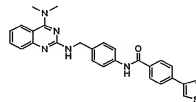
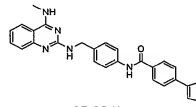
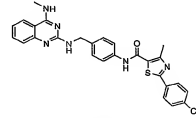
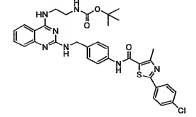
| Example No. | Structure  | ESI-MS        | Retention Time (min) |
|-------------|--|---------------|----------------------|
| 3137        | <br><chem>COc1cc(N)cc(Cl)c1C(=O)NCC1CCCCC1Nc2nc3ccccc3n2C</chem><br>$2\text{CF}_3\text{CO}_2\text{H}$ | 483.2 (M + H) | 2.83                 |
| 3138        | <br><chem>c1ccccc1-c2cc(C(=O)NCC1CCCCC1Nc3nc4ccccc4n3C)s2</chem><br>$\text{CF}_3\text{CO}_2\text{H}$  | 487.4 (M+2H+) | 3.40                 |
| 3139        | <br><chem>Cc1nc2ccccc2n1C(=O)NCC1CCCCC1Nc3nc4ccccc4n3C</chem><br>$\text{CF}_3\text{CO}_2\text{H}$     | 445.6 (M + H) | 2.36                 |
| 3140        | <br><chem>Nc1cc(Cl)c(C(=O)NCC1CCCCC1Nc2nc3ccccc3n2C)cc1</chem><br>$2\text{CF}_3\text{CO}_2\text{H}$   | 453.2 (M + H) | 2.46                 |
| 3141        | <br><chem>COc1cc(OC)c(C(=O)NCC1CCCCC1Nc2nc3ccccc3n2C)cc1</chem><br>$\text{CF}_3\text{CO}_2\text{H}$   | 478.4 (M + H) | 2.77                 |
| 3142        | <br><chem>Oc1cc(I)c(C(=O)NCC1CCCCC1Nc2nc3ccccc3n2C)cc1</chem><br>$\text{CF}_3\text{CO}_2\text{H}$   | 672.2 (M + H) | 3.92                 |

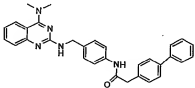
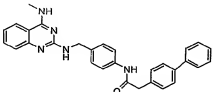
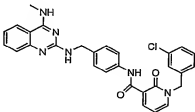
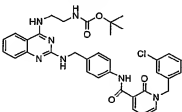
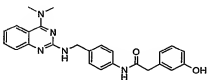
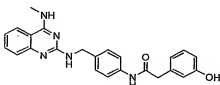
| Example No. | Structure   | ESI-MS        | Retention Time (min) |
|-------------|---|---------------|----------------------|
| 3143        | <br>$\text{CF}_3\text{CO}_2\text{H}$   | 576.2 (M + H) | 3.71                 |
| 3144        | <br>$2\text{CF}_3\text{CO}_2\text{H}$  | 421.2 (M + H) | 2.01                 |
| 3145        | <br>$\text{CF}_3\text{CO}_2\text{H}$   | 494.4 (M + H) | 2.77                 |
| 3146        | <br>$2\text{CF}_3\text{CO}_2\text{H}$  | 405.6 (M + H) | 1.99                 |
| 3147        | <br>$\text{CF}_3\text{CO}_2\text{H}$   | 488.4 (M + H) | 3.13                 |
| 3148        | <br>$\text{CF}_3\text{CO}_2\text{H}$ | 430.4 (M + H) | 2.91                 |

| Example No. | Structure   | ESI-MS        | Retention Time (min) |
|-------------|---|---------------|----------------------|
| 3149        | <br>$2\text{CF}_3\text{CO}_2\text{H}$  | 459.4 (M + H) | 2.47                 |
| 3150        | <br>$\text{CF}_3\text{CO}_2\text{H}$   | 486.6 (M + H) | 2.93                 |
| 3151        | <br>$\text{CF}_3\text{CO}_2\text{H}$   | 474.4 (M + H) | 3.03                 |
| 3152        | <br>$\text{CF}_3\text{CO}_2\text{H}$   | 465.2 (M + H) | 3.13                 |
| 3153        | <br>$2\text{CF}_3\text{CO}_2\text{H}$  | 483.4 (M + H) | 2.67                 |
| 3154        | <br>$\text{CF}_3\text{CO}_2\text{H}$ | 556.4 (M + H) | 2.84                 |

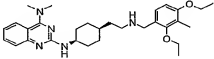
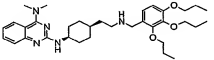
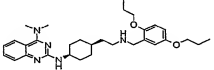
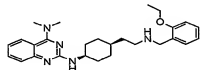
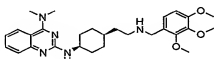
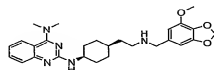


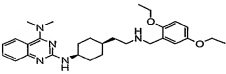
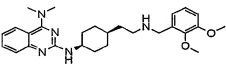
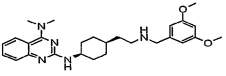
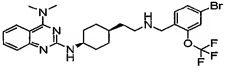
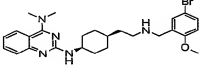
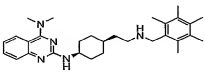
| Example No. | Structure   | ESI-MS        | Retention Time (min) |
|-------------|---|---------------|----------------------|
| 3161        | <br><chem>CC1=NC2=CC=CC=C2N1N(C)CC3CCCCC3NC(=O)c4oc(cc4C(F)(F)F)c5ccc(Cl)cc5</chem><br>$\text{CF}_3\text{CO}_2\text{H}$      | 572.4 (M + H) | 3.71                 |
| 3162        | <br><chem>Cc1nc2ccccc2n1NCc3ccc(NC(=O)c4ccc(cc4)cc5ccccc5)cc3</chem><br>$\text{CF}_3\text{CO}_2\text{H}$                     | 460.2 (M + H) | 3.80                 |
| 3163        | <br><chem>CC(C)(C)OC(=O)NCc1nc2ccccc2n1NCc3ccc(NC(=O)c4ccc(cc4)cc5ccccc5)cc3</chem><br>$\text{CF}_3\text{CO}_2\text{H}$      | 589.2 (M + H) | 4.00                 |
| 3164        | <br><chem>Cc1nc2ccccc2n1NCc3ccc(NC(=O)c4ccc(cc4)cc5ccc(F)cc5)cc3</chem><br>$\text{CF}_3\text{CO}_2\text{H}$                  | 492.2 (M + H) | 3.90                 |
| 3165        | <br><chem>Cc1nc2ccccc2n1NCc3ccc(NC(=O)c4ccc(cc4)cc5ccc(F)cc5)cc3</chem><br>$\text{CF}_3\text{CO}_2\text{H}$                  | 478.2 (M + H) | 3.80                 |
| 3166        | <br><chem>CC(C)(C)OC(=O)NCc1nc2ccccc2n1NCc3ccc(NC(=O)c4ccc(cc4)cc5ccc(F)cc5)cc3</chem><br>$\text{CF}_3\text{CO}_2\text{H}$ | 607.6 (M + H) | 4.00                 |

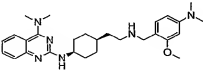
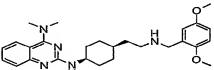
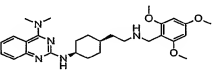
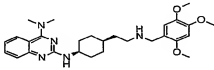
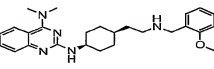
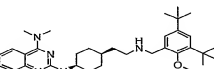
| Example No. | Structure  | ESI-MS        | Retention Time (min) |
|-------------|--|---------------|----------------------|
| 3167        |  <p>CF<sub>3</sub>CO<sub>2</sub>H</p>   | 504.2 (M + H) | 3.40                 |
| 3168        |  <p>CF<sub>3</sub>CO<sub>2</sub>H</p>   | 506.2 (M + H) | 3.90                 |
| 3169        |  <p>CF<sub>3</sub>CO<sub>2</sub>H</p>   | 480.2 (M + H) | 3.80                 |
| 3170        |  <p>CF<sub>3</sub>CO<sub>2</sub>H</p>   | 466.2 (M + H) | 3.70                 |
| 3171        |  <p>CF<sub>3</sub>CO<sub>2</sub>H</p>   | 515.2 (M + H) | 3.90                 |
| 3172        |  <p>CF<sub>3</sub>CO<sub>2</sub>H</p> | 644.2 (M + H) | 4.10                 |

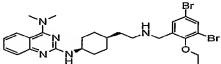
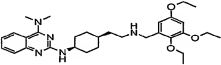
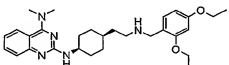
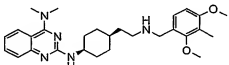
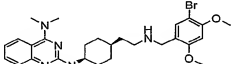
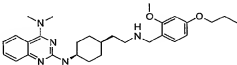
| Example No. | Structure   | ESI-MS        | Retention Time (min) |
|-------------|---|---------------|----------------------|
| 3173        | <br><chem>CC1=NC2=C(N1)N=CN=C2C3=CC=C(C=C3)N4=CC=C(C=C4)NC(=O)CC5=CC=CC=C5</chem><br>$\text{CF}_3\text{CO}_2\text{H}$  | 488.2 (M + H) | 3.90                 |
| 3174        | <br><chem>CC1=NC2=C(N1)N=CN=C2C3=CC=C(C=C3)N4=CC=C(C=C4)NC(=O)CC5=CC=CC=C5</chem><br>$\text{CF}_3\text{CO}_2\text{H}$  | 474.4 (M + H) | 3.80                 |
| 3175        | <br><chem>CC1=NC2=C(N1)N=CN=C2C3=CC=C(C=C3)N4=CC=C(C=C4)NC(=O)CC5=CC=C(C=C5)N6C(=O)C7=CC=C(C=C7)N(C6)C8=CC=CC=C8Cl</chem><br>$\text{CF}_3\text{CO}_2\text{H}$                        | 525.4 (M + H) | 3.70                 |
| 3176        | <br><chem>CC(C)(C)OC(=O)NC1=CC=C(C=C1)N2=CC=C(C=C2)N3=CC=C(C=C3)N4=CC=C(C=C4)NC(=O)CC5=CC=C(C=C5)N6C(=O)C7=CC=C(C=C7)N(C6)C8=CC=C(C=C8)Cl</chem><br>$\text{CF}_3\text{CO}_2\text{H}$ | 654.2 (M + H) | 3.90                 |
| 3177        | <br><chem>CC1=NC2=C(N1)N=CN=C2C3=CC=C(C=C3)N4=CC=C(C=C4)NC(=O)CC5=CC=C(C=C5)O</chem><br>$\text{CF}_3\text{CO}_2\text{H}$   | 428.2 (M + H) | 3.10                 |
| 3178        | <br><chem>CC1=NC2=C(N1)N=CN=C2C3=CC=C(C=C3)N4=CC=C(C=C4)NC(=O)CC5=CC=C(C=C5)O</chem><br>$\text{CF}_3\text{CO}_2\text{H}$   | 414.4 (M + H) | 2.90                 |

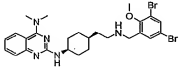
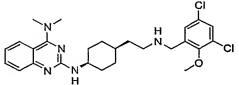
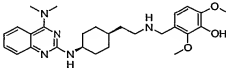
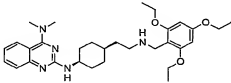
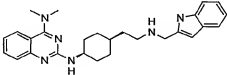
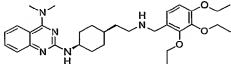


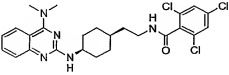
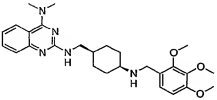
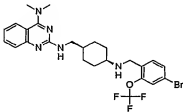
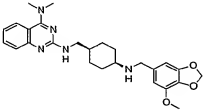
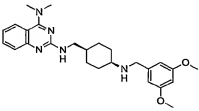
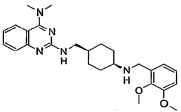
| Example No. | Structure  | ESI-MS        | Retention Time (min) |
|-------------|--|---------------|----------------------|
| 3179        | <br>$2\text{CF}_3\text{CO}_2\text{H}$   | 506.4 (M + H) | 3.04                 |
| 3180        | <br>$2\text{CF}_3\text{CO}_2\text{H}$   | 578.8 (M + H) | 3.50                 |
| 3181        | <br>$2\text{CF}_3\text{CO}_2\text{H}$   | 520.6 (M + H) | 3.19                 |
| 3182        | <br>$2\text{CF}_3\text{CO}_2\text{H}$   | 448.4 (M + H) | 2.80                 |
| 3183        | <br>$2\text{CF}_3\text{CO}_2\text{H}$   | 494.6 (M + H) | 2.66                 |
| 3184        | <br>$2\text{CF}_3\text{CO}_2\text{H}$ | 478.4 (M + H) | 2.66                 |

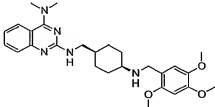
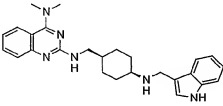
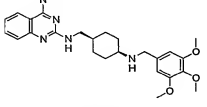
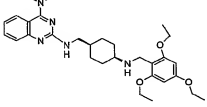
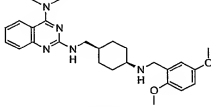
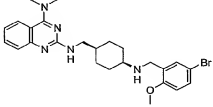
| Example No. | Structure  | ESI-MS        | Retention Time (min) |
|-------------|--|---------------|----------------------|
| 3185        | <br>$2\text{CF}_3\text{CO}_2\text{H}$   | 492.6 (M + H) | 2.94                 |
| 3186        | <br>$2\text{CF}_3\text{CO}_2\text{H}$   | 464.4 (M + H) | 2.65                 |
| 3187        | <br>$2\text{CF}_3\text{CO}_2\text{H}$   | 464.4 (M + H) | 2.68                 |
| 3188        | <br>$2\text{CF}_3\text{CO}_2\text{H}$   | 566.4 (M + H) | 3.03                 |
| 3189        | <br>$2\text{CF}_3\text{CO}_2\text{H}$   | 512.6 (M + H) | 2.85                 |
| 3190        | <br>$2\text{CF}_3\text{CO}_2\text{H}$ | 474.4 (M + H) | 3.09                 |

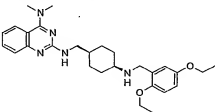
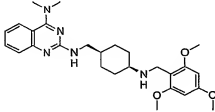
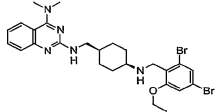
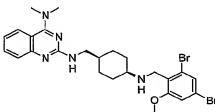
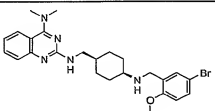
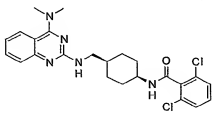
| Example No. | Structure   | ESI-MS        | Retention Time (min) |
|-------------|---|---------------|----------------------|
| 3191        | <br>$3CF_3CO_2H$   | 477.4 (M + H) | 2.51                 |
| 3192        | <br>$2CF_3CO_2H$   | 464.4 (M + H) | 2.67                 |
| 3193        | <br>$2CF_3CO_2H$   | 494.6 (M + H) | 2.78                 |
| 3194        | <br>$2CF_3CO_2H$   | 494.6 (M + H) | 2.60                 |
| 3195        | <br>$2CF_3CO_2H$   | 434.6 (M + H) | 2.67                 |
| 3196        | <br>$2CF_3CO_2H$ | 546.4 (M + H) | 4.30                 |

| Example No. | Structure   | ESI-MS        | Retention Time (min) |
|-------------|---|---------------|----------------------|
| 3197        | <br><chem>CC1=CC=C2N=CN=C2N1C3=CC=CC=C3N3CCCCC3CCNCC4=CC(=C(C=C4)Br)OC</chem><br>$2\text{CF}_3\text{CO}_2\text{H}$             | 606.6 (M + H) | 3.95                 |
| 3198        | <br><chem>CC1=CC=C2N=CN=C2N1C3=CC=CC=C3N3CCCCC3CCNCC4=CC(=C(C=C4)OC)OC</chem><br>$2\text{CF}_3\text{CO}_2\text{H}$             | 536.6 (M + H) | 3.83                 |
| 3199        | <br><chem>CC1=CC=C2N=CN=C2N1C3=CC=CC=C3N3CCCCC3CCNCC4=CC(=CC=C4)OCOC</chem><br>$2\text{CF}_3\text{CO}_2\text{H}$               | 492.4 (M + H) | 2.97                 |
| 3200        | <br><chem>CC1=CC=C2N=CN=C2N1C3=CC=CC=C3N3CCCCC3CCNCC4=CC(=C(C=C4)OC)C(=C(C=C4)OC)C</chem><br>$2\text{CF}_3\text{CO}_2\text{H}$ | 478.4 (M + H) | 2.79                 |
| 3201        | <br><chem>CC1=CC=C2N=CN=C2N1C3=CC=CC=C3N3CCCCC3CCNCC4=CC(=C(C=C4)Br)OCOC</chem><br>$2\text{CF}_3\text{CO}_2\text{H}$           | 542.0 (M + H) | 2.85                 |
| 3202        | <br><chem>CC1=CC=C2N=CN=C2N1C3=CC=CC=C3N3CCCCC3CCNCC4=CC(=CC=C4)OCOC</chem><br>$2\text{CF}_3\text{CO}_2\text{H}$             | 492.6 (M + H) | 2.81                 |

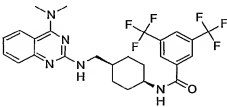
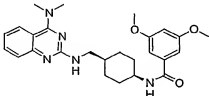
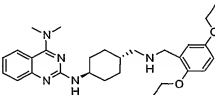
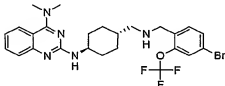
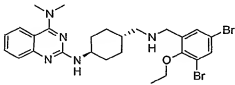
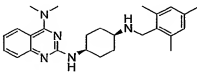
| Example No. | Structure  | ESI-MS        | Retention Time (min) |
|-------------|--|---------------|----------------------|
| 3203        | <br>$2\text{CF}_3\text{CO}_2\text{H}$   | 590.4 (M + H) | 3.02                 |
| 3204        | <br>$2\text{CF}_3\text{CO}_2\text{H}$   | 502.2 (M + H) | 2.91                 |
| 3205        | <br>$2\text{CF}_3\text{CO}_2\text{H}$   | 480.4 (M + H) | 2.51                 |
| 3206        | <br>$2\text{CF}_3\text{CO}_2\text{H}$   | 536.4 (M + H) | 3.21                 |
| 3207        | <br>$3\text{CF}_3\text{CO}_2\text{H}$   | 443.6 (M + H) | 2.66                 |
| 3208        | <br>$2\text{CF}_3\text{CO}_2\text{H}$ | 536.4 (M + H) | 3.08                 |

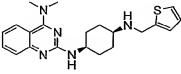
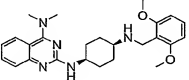
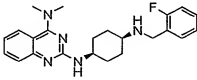
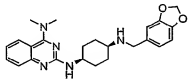
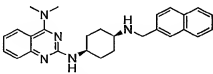
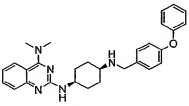
| Example No. | Structure   | ESI-MS        | Retention Time (min) |
|-------------|---|---------------|----------------------|
| 3209        | <br><chem>CC1=CN(C)N=C1N2C=NC(=C2)N3CCCCC3CCNC(=O)c4cc(Cl)cc(Cl)c4</chem><br>$2\text{CF}_3\text{CO}_2\text{H}$         | 520.0 (M + H) | 3.51                 |
| 3210        | <br><chem>CC1=CN(C)N=C1N2C=NC(=C2)N3CCCCC3CCNC(=O)Cc4cc(OC)c(OC)c4</chem><br>$2\text{CF}_3\text{CO}_2\text{H}$         | 480.4 (M + H) | 2.58                 |
| 3211        | <br><chem>CC1=CN(C)N=C1N2C=NC(=C2)N3CCCCC3CCNC(=O)Cc4cc(Br)cc(OC(F)(F)F)c4</chem><br>$2\text{CF}_3\text{CO}_2\text{H}$ | 552.0 (M + H) | 3.11                 |
| 3212        | <br><chem>CC1=CN(C)N=C1N2C=NC(=C2)N3CCCCC3CCNC(=O)Cc4c5cc(OC)OCO5</chem><br>$2\text{CF}_3\text{CO}_2\text{H}$          | 464.4 (M + H) | 3.22                 |
| 3213        | <br><chem>CC1=CN(C)N=C1N2C=NC(=C2)N3CCCCC3CCNC(=O)Cc4cc(OC)cc(OC)c4</chem><br>$2\text{CF}_3\text{CO}_2\text{H}$        | 450.4 (M + H) | 2.70                 |
| 3214        | <br><chem>CC1=CN(C)N=C1N2C=NC(=C2)N3CCCCC3CCNC(=O)Cc4cc(OC)c(OC)c4</chem><br>$2\text{CF}_3\text{CO}_2\text{H}$       | 450.4 (M + H) | 2.58                 |

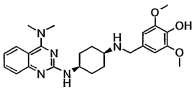
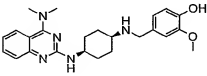
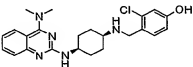
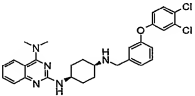
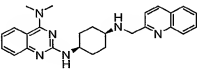
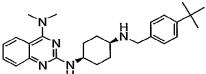
| Example No. | Structure  | ESI-MS        | Retention Time (min) |
|-------------|--|---------------|----------------------|
| 3215        | <br>$2\text{CF}_3\text{CO}_2\text{H}$   | 480.4 (M + H) | 2.73                 |
| 3216        | <br>$3\text{CF}_3\text{CO}_2\text{H}$   | 429.4 (M + H) | 3.29                 |
| 3217        | <br>$2\text{CF}_3\text{CO}_2\text{H}$   | 480.2 (M + H) | 2.78                 |
| 3218        | <br>$2\text{CF}_3\text{CO}_2\text{H}$   | 522.4 (M + H) | 3.77                 |
| 3219        | <br>$2\text{CF}_3\text{CO}_2\text{H}$   | 450.2 (M + H) | 2.57                 |
| 3220        | <br>$2\text{CF}_3\text{CO}_2\text{H}$ | 498.0 (M + H) | 2.97                 |

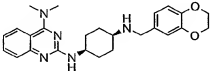
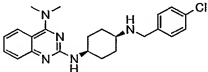
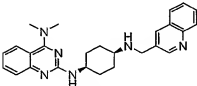
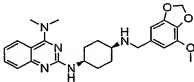
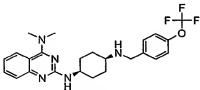
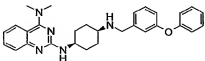
| Example No. | Structure  | ESI-MS        | Retention Time (min) |
|-------------|--|---------------|----------------------|
| 3221        |  <p>2CF<sub>3</sub>CO<sub>2</sub>H</p>  | 478.4 (M + H) | 3.17                 |
| 3222        |  <p>2CF<sub>3</sub>CO<sub>2</sub>H</p>  | 480.0 (M + H) | 3.08                 |
| 3223        |  <p>2CF<sub>3</sub>CO<sub>2</sub>H</p>  | 590.2 (M + H) | 4.20                 |
| 3224        |  <p>2CF<sub>3</sub>CO<sub>2</sub>H</p>  | 576.4 (M + H) | 3.95                 |
| 3225        |  <p>2CF<sub>3</sub>CO<sub>2</sub>H</p>  | 512.4 (M + H) | 3.86                 |
| 3226        |  <p>CF<sub>3</sub>CO<sub>2</sub>H</p> | 472.4 (M + H) | 3.07                 |



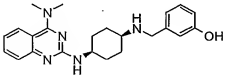
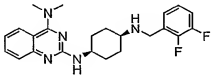
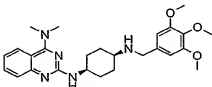
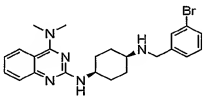
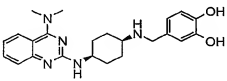
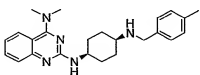
| Example No. | Structure  | ESI-MS        | Retention Time (min) |
|-------------|--|---------------|----------------------|
| 3227        | <br>$\text{CF}_3\text{CO}_2\text{H}$    | 540.6 (M + H) | 3.75                 |
| 3228        | <br>$\text{CF}_3\text{CO}_2\text{H}$    | 464.4 (M + H) | 3.07                 |
| 3229        | <br>$2\text{CF}_3\text{CO}_2\text{H}$   | 478.4 (M + H) | 3.40                 |
| 3230        | <br>$2\text{CF}_3\text{CO}_2\text{H}$   | 552.6 (M + H) | 3.50                 |
| 3231        | <br>$2\text{CF}_3\text{CO}_2\text{H}$   | 590.2 (M + H) | 3.60                 |
| 3232        | <br>$2\text{CF}_3\text{CO}_2\text{H}$ | 418.6 (M + H) | 3.25                 |

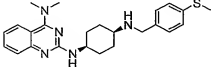
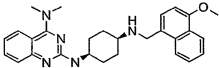
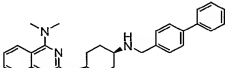
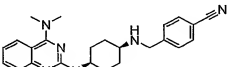
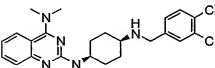
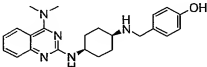
| Example No. | Structure  | ESI-MS        | Retention Time (min) |
|-------------|--|---------------|----------------------|
| 3233        | <br>$2\text{CF}_3\text{CO}_2\text{H}$   | 382.2 (M + H) | 2.67                 |
| 3234        | <br>$2\text{CF}_3\text{CO}_2\text{H}$   | 436.4 (M + H) | 3.05                 |
| 3235        | <br>$2\text{CF}_3\text{CO}_2\text{H}$   | 394.4 (M + H) | 2.75                 |
| 3236        | <br>$2\text{CF}_3\text{CO}_2\text{H}$   | 420.4 (M + H) | 2.82                 |
| 3237        | <br>$2\text{CF}_3\text{CO}_2\text{H}$   | 426.4 (M + H) | 3.17                 |
| 3238        | <br>$2\text{CF}_3\text{CO}_2\text{H}$ | 468.4 (M + H) | 3.44                 |

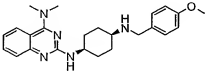
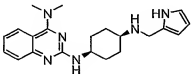
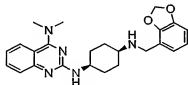
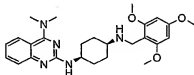
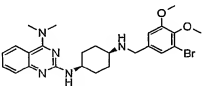
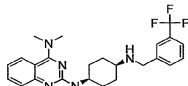
| Example No. | Structure  | ESI-MS        | Retention Time (min) |
|-------------|--|---------------|----------------------|
| 3239        | <br>$2\text{CF}_3\text{CO}_2\text{H}$   | 452.2 (M + H) | 2.69                 |
| 3240        | <br>$2\text{CF}_3\text{CO}_2\text{H}$   | 436.4 (M + H) | 2.80                 |
| 3241        | <br>$2\text{CF}_3\text{CO}_2\text{H}$   | 426.2 (M + H) | 2.79                 |
| 3242        | <br>$2\text{CF}_3\text{CO}_2\text{H}$   | 536.4 (M + H) | 3.75                 |
| 3243        | <br>$3\text{CF}_3\text{CO}_2\text{H}$   | 427.2 (M + H) | 2.95                 |
| 3244        | <br>$2\text{CF}_3\text{CO}_2\text{H}$ | 432.4 (M + H) | 3.41                 |

| Example No. | Structure  | ESI-MS        | Retention Time (min) |
|-------------|--|---------------|----------------------|
| 3245        | <br>$2\text{CF}_3\text{CO}_2\text{H}$   | 434.2 (M + H) | 2.84                 |
| 3246        | <br>$2\text{CF}_3\text{CO}_2\text{H}$   | 410.2 (M + H) | 3.02                 |
| 3247        | <br>$3\text{CF}_3\text{CO}_2\text{H}$   | 427.4 (M + H) | 2.61                 |
| 3248        | <br>$2\text{CF}_3\text{CO}_2\text{H}$   | 450.4 (M + H) | 2.91                 |
| 3249        | <br>$2\text{CF}_3\text{CO}_2\text{H}$   | 460.4 (M + H) | 3.19                 |
| 3250        | <br>$2\text{CF}_3\text{CO}_2\text{H}$ | 468.4 (M + H) | 2.79                 |

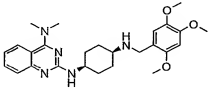
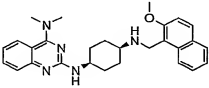
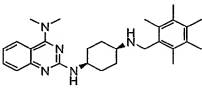
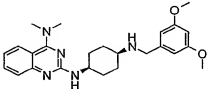
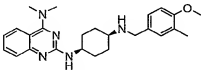
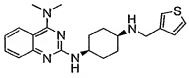
| Example No. | Structure        | ESI-MS        | Retention Time (min) |
|-------------|------------------|---------------|----------------------|
| 3251        | <br>$2CF_3CO_2H$ | 394.4 (M + H) | 2.83                 |
| 3252        | <br>$2CF_3CO_2H$ | 454.2 (M + H) | 3.08                 |
| 3253        | <br>$2CF_3CO_2H$ | 392.4 (M + H) | 2.73                 |
| 3254        | <br>$2CF_3CO_2H$ | 450.4 (M + H) | 2.92                 |
| 3255        | <br>$3CF_3CO_2H$ | 510.4 (M + H) | 3.17                 |
| 3256        | <br>$2CF_3CO_2H$ | 428.2 (M + H) | 3.08                 |

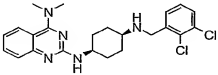
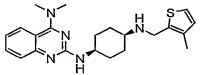
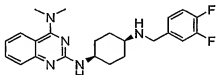
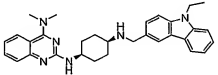
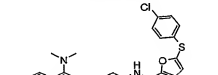
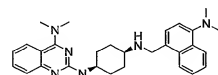
| Example No. | Structure  | ESI-MS        | Retention Time (min) |
|-------------|--|---------------|----------------------|
| 3257        | <br><chem>CN(C)c1nc2c(ncn2C1NCC3CCCCC3NCc4ccc(O)cc4)cc5ccccc15</chem><br>$2\text{CF}_3\text{CO}_2\text{H}$          | 392.4 (M + H) | 2.63                 |
| 3258        | <br><chem>CN(C)c1nc2c(ncn2C1NCC3CCCCC3NCc4cc(F)c(F)cc4)cc5ccccc15</chem><br>$2\text{CF}_3\text{CO}_2\text{H}$       | 412.2 (M + H) | 2.83                 |
| 3259        | <br><chem>CN(C)c1nc2c(ncn2C1NCC3CCCCC3NCc4cc(OC)c(OC)c(OC)c4)cc5ccccc15</chem><br>$2\text{CF}_3\text{CO}_2\text{H}$ | 466.4 (M + H) | 2.89                 |
| 3260        | <br><chem>CN(C)c1nc2c(ncn2C1NCC3CCCCC3NCc4ccc(Br)cc4)cc5ccccc15</chem><br>$2\text{CF}_3\text{CO}_2\text{H}$         | 454.0 (M + H) | 3.05                 |
| 3261        | <br><chem>CN(C)c1nc2c(ncn2C1NCC3CCCCC3NCc4cc(O)c(O)cc4)cc5ccccc15</chem><br>$2\text{CF}_3\text{CO}_2\text{H}$       | 408.2 (M + H) | 2.53                 |
| 3262        | <br><chem>CN(C)c1nc2c(ncn2C1NCC3CCCCC3NCc4ccc(C)cc4)cc5ccccc15</chem><br>$2\text{CF}_3\text{CO}_2\text{H}$        | 390.4 (M + H) | 2.92                 |

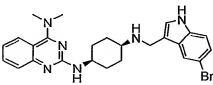
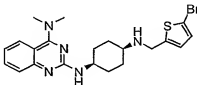
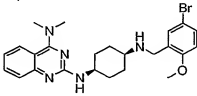
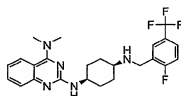
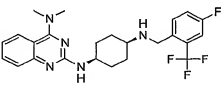
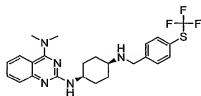
| Example No. | Structure  | ESI-MS        | Retention Time (min) |
|-------------|--|---------------|----------------------|
| 3263        | <br><chem>CC1=NC2=CC=CC=C2N1N(C)C3=CC=C(C)N3C4CCCCC4NC5=CC=C(C)C=C5</chem><br>$2\text{CF}_3\text{CO}_2\text{H}$ | 422.2 (M + H) | 3.05                 |
| 3264        | <br><chem>COc1ccc(cc1)CN[C@H]2CCCC[C@H]2Nc3nc4ccccc4n3C</chem><br>$2\text{CF}_3\text{CO}_2\text{H}$             | 456.4 (M + H) | 3.25                 |
| 3265        | <br><chem>c1ccc(cc1)CN[C@H]2CCCC[C@H]2Nc3nc4ccccc4n3C</chem><br>$2\text{CF}_3\text{CO}_2\text{H}$               | 452.2 (M + H) | 3.37                 |
| 3266        | <br><chem>N#Cc1ccc(cc1)CN[C@H]2CCCC[C@H]2Nc3nc4ccccc4n3C</chem><br>$2\text{CF}_3\text{CO}_2\text{H}$            | 401.2 (M + H) | 2.76                 |
| 3267        | <br><chem>Clc1cc(Cl)ccc1CN[C@H]2CCCC[C@H]2Nc3nc4ccccc4n3C</chem><br>$2\text{CF}_3\text{CO}_2\text{H}$           | 444.4 (M + H) | 3.17                 |
| 3268        | <br><chem>Oc1ccc(cc1)CN[C@H]2CCCC[C@H]2Nc3nc4ccccc4n3C</chem><br>$2\text{CF}_3\text{CO}_2\text{H}$            | 392.4 (M + H) | 2.61                 |

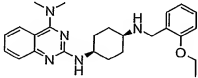
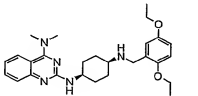
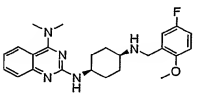
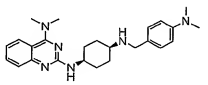
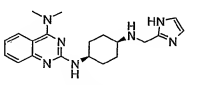
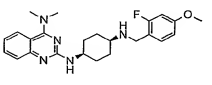
| Example No. | Structure  | ESI-MS        | Retention Time (min) |
|-------------|--|---------------|----------------------|
| 3269        | <br>$2\text{CF}_3\text{CO}_2\text{H}$   | 406.4 (M + H) | 2.86                 |
| 3270        | <br>$3\text{CF}_3\text{CO}_2\text{H}$   | 365.4 (M + H) | 2.61                 |
| 3271        | <br>$2\text{CF}_3\text{CO}_2\text{H}$   | 420.4 (M + H) | 2.83                 |
| 3272        | <br>$2\text{CF}_3\text{CO}_2\text{H}$   | 466.4 (M + H) | 3.10                 |
| 3273        | <br>$2\text{CF}_3\text{CO}_2\text{H}$   | 514.4 (M + H) | 3.13                 |
| 3274        | <br>$2\text{CF}_3\text{CO}_2\text{H}$ | 444.4 (M + H) | 3.17                 |

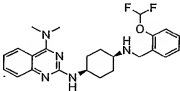
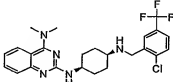
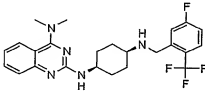
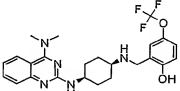
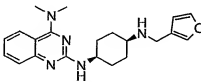
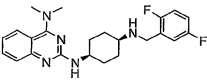


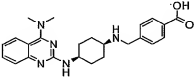
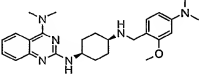
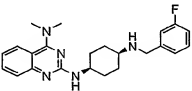
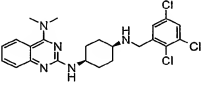
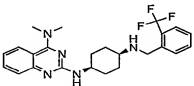
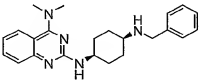
| Example No. | Structure  | ESI-MS        | Retention Time (min) |
|-------------|--|---------------|----------------------|
| 3275        | <br>$2\text{CF}_3\text{CO}_2\text{H}$   | 466.4 (M + H) | 2.86                 |
| 3276        | <br>$2\text{CF}_3\text{CO}_2\text{H}$   | 456.2 (M + H) | 3.22                 |
| 3277        | <br>$2\text{CF}_3\text{CO}_2\text{H}$   | 446.6 (M + H) | 3.45                 |
| 3278        | <br>$2\text{CF}_3\text{CO}_2\text{H}$   | 436.4 (M + H) | 2.95                 |
| 3279        | <br>$2\text{CF}_3\text{CO}_2\text{H}$   | 420.2 (M + H) | 3.03                 |
| 3280        | <br>$2\text{CF}_3\text{CO}_2\text{H}$ | 382.4 (M + H) | 2.72                 |

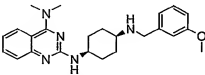
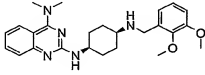
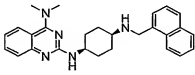
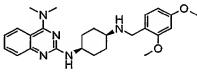
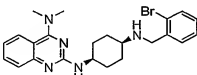
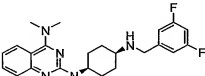
| Example No. | Structure  | ESI-MS        | Retention Time (min) |
|-------------|--|---------------|----------------------|
| 3281        | <br>$2\text{CF}_3\text{CO}_2\text{H}$   | 444.4 (M + H) | 3.07                 |
| 3282        | <br>$2\text{CF}_3\text{CO}_2\text{H}$   | 396.2 (M + H) | 2.79                 |
| 3283        | <br>$2\text{CF}_3\text{CO}_2\text{H}$   | 412.4 (M + H) | 2.95                 |
| 3284        | <br>$32\text{CF}_3\text{CO}_2\text{H}$  | 493.4 (M + H) | 3.57                 |
| 3285        | <br>$2\text{CF}_3\text{CO}_2\text{H}$   | 508.2 (M + H) | 3.52                 |
| 3286        | <br>$2\text{CF}_3\text{CO}_2\text{H}$ | 469.6 (M + H) | 2.76                 |

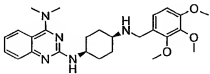
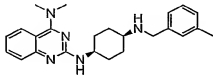
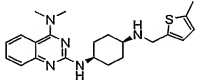
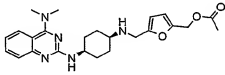
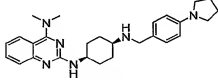
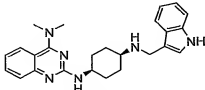
| Example No. | Structure  | ESI-MS        | Retention Time (min) |
|-------------|--|---------------|----------------------|
| 3287        | <br>$3\text{CF}_3\text{CO}_2\text{H}$   | 493.2 (M + H) | 3.17                 |
| 3288        | <br>$2\text{CF}_3\text{CO}_2\text{H}$   | 460.2 (M + H) | 2.95                 |
| 3289        | <br>$2\text{CF}_3\text{CO}_2\text{H}$   | 484.2 (M + H) | 3.14                 |
| 3290        | <br>$2\text{CF}_3\text{CO}_2\text{H}$   | 462.2 (M + H) | 3.11                 |
| 3291        | <br>$2\text{CF}_3\text{CO}_2\text{H}$   | 462.2 (M + H) | 3.11                 |
| 3292        | <br>$2\text{CF}_3\text{CO}_2\text{H}$ | 476.4 (M + H) | 3.39                 |

| Example No. | Structure  | ESI-MS        | Retention Time (min) |
|-------------|--|---------------|----------------------|
| 3293        | <br><chem>CCOC1=CC=C(C=C1)CN[C@H]2CCCC[C@H]2Nc3nc4c(ncn3C)C5=CC=CC=C5</chem><br>$2\text{CF}_3\text{CO}_2\text{H}$   | 420.4 (M + H) | 3.05                 |
| 3294        | <br><chem>COc1cc(OC)cc(CN[C@H]2CCCC[C@H]2Nc3nc4c(ncn3C)C5=CC=CC=C5)c1</chem><br>$2\text{CF}_3\text{CO}_2\text{H}$   | 464.2 (M + H) | 3.21                 |
| 3295        | <br><chem>COc1cc(F)ccc(CN[C@H]2CCCC[C@H]2Nc3nc4c(ncn3C)C5=CC=CC=C5)c1</chem><br>$2\text{CF}_3\text{CO}_2\text{H}$   | 424.2 (M + H) | 2.94                 |
| 3296        | <br><chem>CN(C)Cc1ccc(CN[C@H]2CCCC[C@H]2Nc3nc4c(ncn3C)C5=CC=CC=C5)cc1</chem><br>$3\text{CF}_3\text{CO}_2\text{H}$   | 419.4 (M + H) | 2.51                 |
| 3297        | <br><chem>C1=CN=C(NC1)CN[C@H]2CCCC[C@H]2Nc3nc4c(ncn3C)C5=CC=CC=C5</chem><br>$3\text{CF}_3\text{CO}_2\text{H}$       | 366.4 (M + H) | 2.26                 |
| 3298        | <br><chem>COc1cc(F)ccc(CN[C@H]2CCCC[C@H]2Nc3nc4c(ncn3C)C5=CC=CC=C5)c1</chem><br>$2\text{CF}_3\text{CO}_2\text{H}$ | 424.2 (M + H) | 2.93                 |

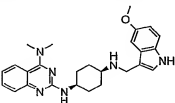
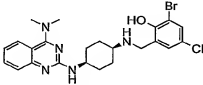
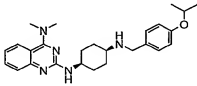
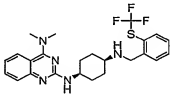
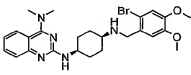
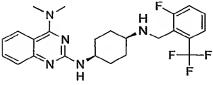
| Example No. | Structure   | ESI-MS        | Retention Time (min) |
|-------------|---|---------------|----------------------|
| 3299        | <br>$2CF_3CO_2H$   | 442.4 (M + H) | 2.97                 |
| 3300        | <br>$2CF_3CO_2H$   | 478.2 (M + H) | 3.19                 |
| 3301        | <br>$2CF_3CO_2H$   | 462.2 (M + H) | 3.05                 |
| 3302        | <br>$2CF_3CO_2H$   | 476.4 (M + H) | 3.20                 |
| 3303        | <br>$2CF_3CO_2H$   | 366.4 (M + H) | 2.64                 |
| 3304        | <br>$2CF_3CO_2H$ | 412.4 (M + H) | 2.85                 |

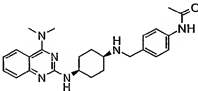
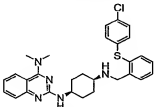
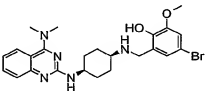
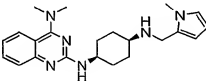
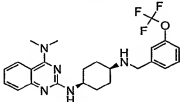
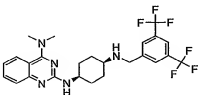
| Example No. | Structure   | ESI-MS        | Retention Time (min) |
|-------------|---|---------------|----------------------|
| 3305        | <br>$2CF_3CO_2H$   | 420.4 (M + H) | 2.67                 |
| 3306        | <br>$3CF_3CO_2H$   | 449.4 (M + H) | 2.74                 |
| 3307        | <br>$2CF_3CO_2H$   | 394.4 (M + H) | 2.86                 |
| 3308        | <br>$2CF_3CO_2H$   | 478.2 (M + H) | 3.38                 |
| 3309        | <br>$2CF_3CO_2H$   | 444.4 (M + H) | 3.09                 |
| 3310        | <br>$2CF_3CO_2H$ | 376.4 (M + H) | 2.82                 |

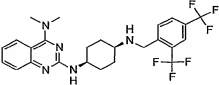
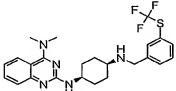
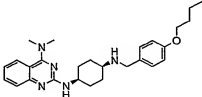
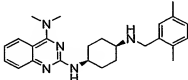
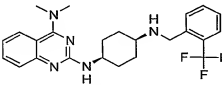
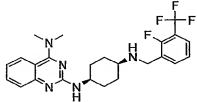
| Example No. | Structure   | ESI-MS        | Retention Time (min) |
|-------------|---|---------------|----------------------|
| 3311        | <br>$2CF_3CO_2H$   | 406.4 (M + H) | 2.87                 |
| 3312        | <br>$2CF_3CO_2H$   | 436.4 (M + H) | 2.91                 |
| 3313        | <br>$2CF_3CO_2H$   | 426.2 (M + H) | 3.13                 |
| 3314        | <br>$2CF_3CO_2H$   | 436.4 (M + H) | 2.99                 |
| 3315        | <br>$2CF_3CO_2H$   | 454.0 (M + H) | 2.97                 |
| 3316        | <br>$2CF_3CO_2H$ | 412.4 (M + H) | 2.92                 |

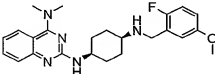
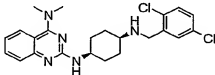
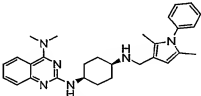
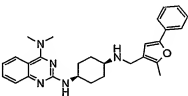
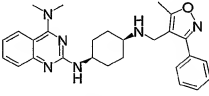
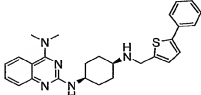
| Example No. | Structure  | ESI-MS        | Retention Time (min) |
|-------------|--|---------------|----------------------|
| 3317        | <br>$2\text{CF}_3\text{CO}_2\text{H}$   | 466.4 (M + H) | 2.95                 |
| 3318        | <br>$2\text{CF}_3\text{CO}_2\text{H}$   | 390.4 (M + H) | 2.95                 |
| 3319        | <br>$2\text{CF}_3\text{CO}_2\text{H}$   | 396.2 (M + H) | 2.89                 |
| 3320        | <br>$2\text{CF}_3\text{CO}_2\text{H}$   | 438.2 (M + H) | 2.76                 |
| 3321        | <br>$3\text{CF}_3\text{CO}_2\text{H}$   | 445.4 (M + H) | 3.16                 |
| 3322        | <br>$3\text{CF}_3\text{CO}_2\text{H}$ | 415.4 (M + H) | 2.96                 |

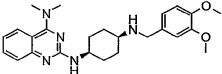
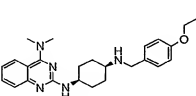
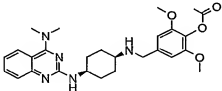
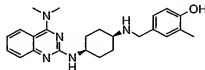
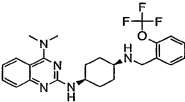
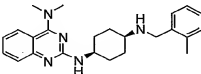


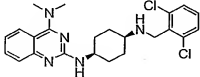
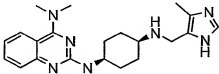
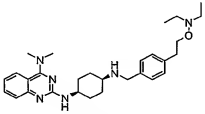
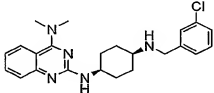
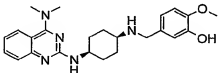
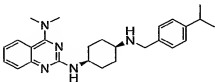
| Example No. | Structure  | ESI-MS        | Retention Time (min) |
|-------------|--|---------------|----------------------|
| 3323        | <br>$3\text{CF}_3\text{CO}_2\text{H}$   | 445.4 (M + H) | 2.96                 |
| 3324        | <br>$2\text{CF}_3\text{CO}_2\text{H}$   | 504.2 (M + H) | 3.11                 |
| 3325        | <br>$2\text{CF}_3\text{CO}_2\text{H}$   | 434.4 (M + H) | 3.17                 |
| 3326        | <br>$2\text{CF}_3\text{CO}_2\text{H}$   | 476.2 (M + H) | 3.27                 |
| 3327        | <br>$2\text{CF}_3\text{CO}_2\text{H}$   | 514.4 (M + H) | 3.07                 |
| 3328        | <br>$2\text{CF}_3\text{CO}_2\text{H}$ | 462.2 (M + H) | 2.99                 |

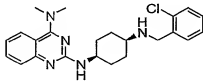
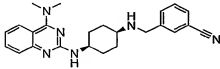
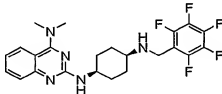
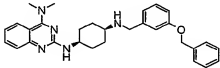
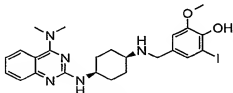
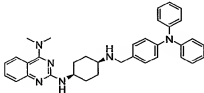
| Example No. | Structure  | ESI-MS        | Retention Time (min) |
|-------------|--|---------------|----------------------|
| 3329        | <br>$2\text{CF}_3\text{CO}_2\text{H}$   | 433.2 (M + H) | 2.63                 |
| 3330        | <br>$2\text{CF}_3\text{CO}_2\text{H}$   | 518.4 (M + H) | 3.63                 |
| 3331        | <br>$2\text{CF}_3\text{CO}_2\text{H}$   | 500.4 (M + H) | 3.09                 |
| 3332        | <br>$3\text{CF}_3\text{CO}_2\text{H}$   | 379.4 (M + H) | 2.77                 |
| 3333        | <br>$2\text{CF}_3\text{CO}_2\text{H}$   | 460.2 (M + H) | 3.31                 |
| 3334        | <br>$2\text{CF}_3\text{CO}_2\text{H}$ | 512.4 (M + H) | 3.51                 |

| Example No. | Structure  | ESI-MS        | Retention Time (min) |
|-------------|--|---------------|----------------------|
| 3335        | <br>$2\text{CF}_3\text{CO}_2\text{H}$   | 512.6 (M + H) | 3.51                 |
| 3336        | <br>$2\text{CF}_3\text{CO}_2\text{H}$   | 476.2 (M + H) | 3.39                 |
| 3337        | <br>$2\text{CF}_3\text{CO}_2\text{H}$   | 448.4 (M + H) | 3.42                 |
| 3338        | <br>$2\text{CF}_3\text{CO}_2\text{H}$   | 404.4 (M + H) | 3.17                 |
| 3339        | <br>$2\text{CF}_3\text{CO}_2\text{H}$   | 444.4 (M + H) | 3.13                 |
| 3340        | <br>$2\text{CF}_3\text{CO}_2\text{H}$ | 462.2 (M + H) | 3.21                 |

| Example No. | Structure  | ESI-MS        | Retention Time (min) |
|-------------|--|---------------|----------------------|
| 3341        | <br>$2\text{CF}_3\text{CO}_2\text{H}$   | 424.2 (M + H) | 2.97                 |
| 3342        | <br>$2\text{CF}_3\text{CO}_2\text{H}$   | 444.6 (M + H) | 3.16                 |
| 3343        | <br>$3\text{CF}_3\text{CO}_2\text{H}$   | 469.4 (M + H) | 3.47                 |
| 3344        | <br>$2\text{CF}_3\text{CO}_2\text{H}$   | 456.4 (M + H) | 3.47                 |
| 3345        | <br>$2\text{CF}_3\text{CO}_2\text{H}$   | 457.4 (M + H) | 3.09                 |
| 3346        | <br>$2\text{CF}_3\text{CO}_2\text{H}$ | 458.2 (M + H) | 3.37                 |

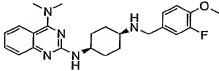
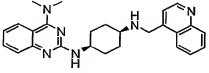
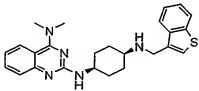
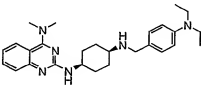
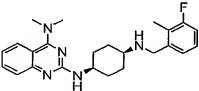
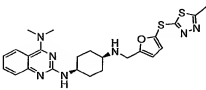
| Example No. | Structure  | ESI-MS        | Retention Time (min) |
|-------------|--|---------------|----------------------|
| 3347        | <br>$2\text{CF}_3\text{CO}_2\text{H}$   | 436.4 (M + H) | 2.83                 |
| 3348        | <br>$2\text{CF}_3\text{CO}_2\text{H}$   | 434.4 (M + H) | 3.30                 |
| 3349        | <br>$2\text{CF}_3\text{CO}_2\text{H}$   | 494.4 (M + H) | 2.98                 |
| 3350        | <br>$2\text{CF}_3\text{CO}_2\text{H}$   | 406.4 (M + H) | 2.80                 |
| 3351        | <br>$2\text{CF}_3\text{CO}_2\text{H}$   | 460.4 (M + H) | 3.20                 |
| 3352        | <br>$2\text{CF}_3\text{CO}_2\text{H}$ | 390.4 (M + H) | 2.97                 |

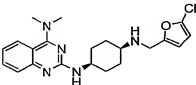
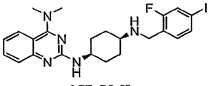
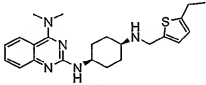
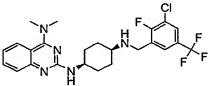
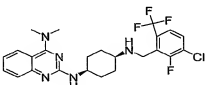
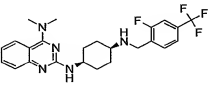
| Example No. | Structure  | ESI-MS        | Retention Time (min) |
|-------------|--|---------------|----------------------|
| 3353        | <br>$2\text{CF}_3\text{CO}_2\text{H}$   | 444.2 (M + H) | 3.01                 |
| 3354        | <br>$3\text{CF}_3\text{CO}_2\text{H}$   | 380.2 (M + H) | 2.27                 |
| 3355        | <br>$2\text{CF}_3\text{CO}_2\text{H}$   | 491.4 (M + H) | 2.55                 |
| 3356        | <br>$2\text{CF}_3\text{CO}_2\text{H}$   | 410.4 (M + H) | 3.05                 |
| 3357        | <br>$2\text{CF}_3\text{CO}_2\text{H}$   | 422.2 (M + H) | 2.69                 |
| 3358        | <br>$2\text{CF}_3\text{CO}_2\text{H}$ | 418.6 (M + H) | 3.36                 |

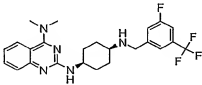
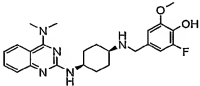
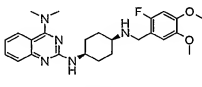
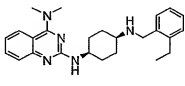
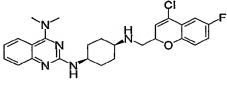
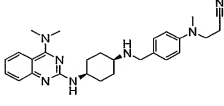
| Example No. | Structure  | ESI-MS        | Retention Time (min) |
|-------------|--|---------------|----------------------|
| 3359        | <br>$2\text{CF}_3\text{CO}_2\text{H}$   | 410.4 (M + H) | 2.97                 |
| 3360        | <br>$2\text{CF}_3\text{CO}_2\text{H}$   | 401.2 (M + H) | 2.81                 |
| 3361        | <br>$2\text{CF}_3\text{CO}_2\text{H}$   | 466.2 (M + H) | 3.01                 |
| 3362        | <br>$2\text{CF}_3\text{CO}_2\text{H}$   | 482.4 (M + H) | 3.43                 |
| 3363        | <br>$2\text{CF}_3\text{CO}_2\text{H}$   | 548.4 (M + H) | 3.03                 |
| 3364        | <br>$3\text{CF}_3\text{CO}_2\text{H}$ | 543.6 (M + H) | 3.95                 |

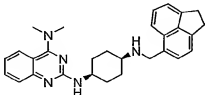
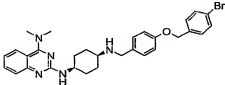
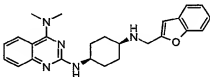
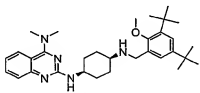
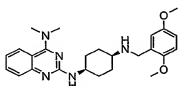
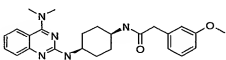


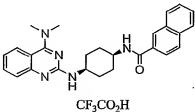
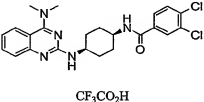
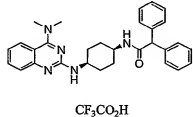
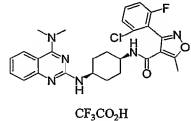
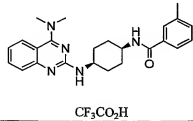
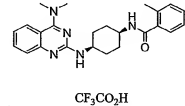


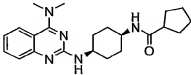
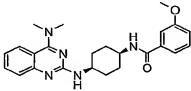
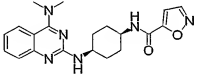
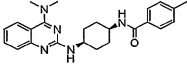
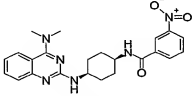
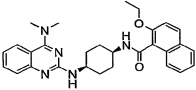
| Example No. | Structure  | ESI-MS        | Retention Time (min) |
|-------------|--|---------------|----------------------|
| 3371        | <br>$2\text{CF}_3\text{CO}_2\text{H}$   | 424.2 (M + H) | 2.96                 |
| 3372        | <br>$3\text{CF}_3\text{CO}_2\text{H}$   | 427.2 (M + H) | 2.53                 |
| 3373        | <br>$2\text{CF}_3\text{CO}_2\text{H}$   | 432.4 (M + H) | 3.12                 |
| 3374        | <br>$3\text{CF}_3\text{CO}_2\text{H}$   | 447.4 (M + H) | 2.45                 |
| 3375        | <br>$2\text{CF}_3\text{CO}_2\text{H}$   | 408.2 (M + H) | 3.02                 |
| 3376        | <br>$2\text{CF}_3\text{CO}_2\text{H}$ | 496.4 (M + H) | 2.81                 |

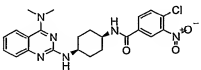
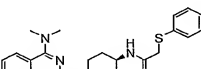
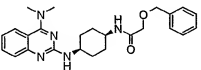
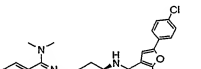
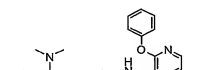
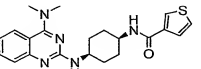
| Example No. | Structure   | ESI-MS        | Retention Time (min) |
|-------------|---|---------------|----------------------|
| 3377        | <br>$2CF_3CO_2H$   | 400.2 (M + H) | 2.81                 |
| 3378        | <br>$2CF_3CO_2H$   | 520.2 (M + H) | 3.14                 |
| 3379        | <br>$2CF_3CO_2H$   | 410.4 (M + H) | 3.12                 |
| 3380        | <br>$2CF_3CO_2H$   | 496.4 (M + H) | 3.40                 |
| 3381        | <br>$2CF_3CO_2H$   | 496.4 (M + H) | 3.17                 |
| 3382        | <br>$2CF_3CO_2H$ | 462.2 (M + H) | 3.19                 |

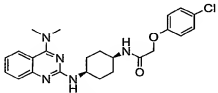
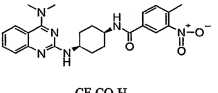
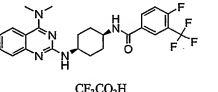
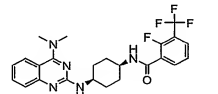
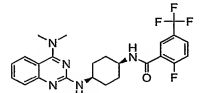
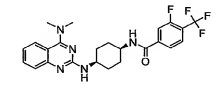
| Example No. | Structure   | ESI-MS        | Retention Time (min) |
|-------------|---|---------------|----------------------|
| 3383        | <br>$2CF_3CO_2H$   | 462.2 (M + H) | 3.28                 |
| 3384        | <br>$2CF_3CO_2H$   | 440.4 (M + H) | 2.74                 |
| 3385        | <br>$2CF_3CO_2H$   | 454.2 (M + H) | 2.89                 |
| 3386        | <br>$2CF_3CO_2H$   | 404.4 (M + H) | 3.09                 |
| 3387        | <br>$2CF_3CO_2H$   | 482.2 (M + H) | 3.29                 |
| 3388        | <br>$3CF_3CO_2H$ | 458.4 (M + H) | 2.99                 |

| Example No. | Structure   | ESI-MS        | Retention Time (min) |
|-------------|---|---------------|----------------------|
| 3389        | <br>$2\text{CF}_3\text{CO}_2\text{H}$  | 452.2 (M + H) | 3.40                 |
| 3390        | <br>$2\text{CF}_3\text{CO}_2\text{H}$  | 560.2 (M + H) | 3.73                 |
| 3391        | <br>$2\text{CF}_3\text{CO}_2\text{H}$  | 416.4 (M + H) | 2.99                 |
| 3392        | <br>$2\text{CF}_3\text{CO}_2\text{H}$  | 518.6 (M + H) | 4.08                 |
| 3393        | <br>$2\text{CF}_3\text{CO}_2\text{H}$  | 436.4 (M + H) | 2.95                 |
| 3394        | <br>$\text{CF}_3\text{CO}_2\text{H}$ | 434.4 (M + H) | 3.30                 |

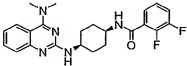
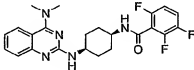
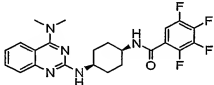
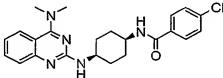
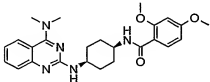
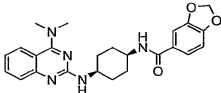
| Example No. | Structure   | ESI-MS        | Retention Time (min) |
|-------------|---|---------------|----------------------|
| 3395        | <br><chem>CC1=C(C2=CC=CC=C2N1)N(C)C3=CC=CC=C3N3C(=O)N(C4=CC=CC=C4C(=O)O)CC5CCCCC5C3</chem><br>$\text{CF}_3\text{CO}_2\text{H}$     | 440.4 (M + H) | 4.26                 |
| 3396        | <br><chem>CC1=C(C2=CC=CC=C2N1)N(C)C3=CC=CC=C3N3C(=O)N(C4=CC(=CC=C4)Cl)CC5CCCCC5C3</chem><br>$\text{CF}_3\text{CO}_2\text{H}$       | 458.2 (M + H) | 4.39                 |
| 3397        | <br><chem>CC1=C(C2=CC=CC=C2N1)N(C)C3=CC=CC=C3N3C(=O)N(C4=CC=CC=C4C(=O)O)CC5CCCCC5C3</chem><br>$\text{CF}_3\text{CO}_2\text{H}$     | 480.4 (M + H) | 4.37                 |
| 3398        | <br><chem>CC1=C(C2=CC=CC=C2N1)N(C)C3=CC=CC=C3N3C(=O)N(C4=CC(=CC=C4)C(=O)O)CC5CCCCC5C3</chem><br>$\text{CF}_3\text{CO}_2\text{H}$   | 523.6 (M + H) | 4.15                 |
| 3399        | <br><chem>CC1=C(C2=CC=CC=C2N1)N(C)C3=CC=CC=C3N3C(=O)N(C4=CC(=CC=C4)C(=O)O)CC5CCCCC5C3</chem><br>$\text{CF}_3\text{CO}_2\text{H}$  | 404.4 (M + H) | 3.46                 |
| 3400        | <br><chem>CC1=C(C2=CC=CC=C2N1)N(C)C3=CC=CC=C3N3C(=O)N(C4=CC(=CC=C4)C(=O)O)CC5CCCCC5C3</chem><br>$\text{CF}_3\text{CO}_2\text{H}$ | 404.4 (M + H) | 3.75                 |

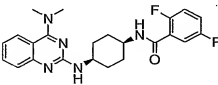
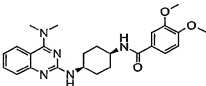
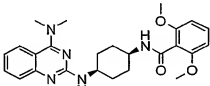
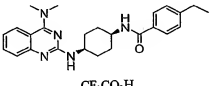
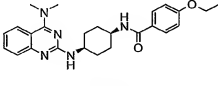
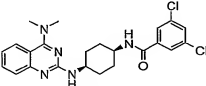
| Example No. | Structure   | ESI-MS        | Retention Time (min) |
|-------------|---|---------------|----------------------|
| 3401        | <br><chem>CC1(C)N2C(=N1)N3C(=N2)NCC3C4CCCC4C(=O)N5CCCC5</chem><br>$\text{CF}_3\text{CO}_2\text{H}$                               | 382.4 (M + H) | 3.65                 |
| 3402        | <br><chem>COc1ccc(cc1)C(=O)N2CCCC2C3C(=N1)N4C(=N3)NCC4C5=CC=CC=C5N1(C)C</chem><br>$\text{CF}_3\text{CO}_2\text{H}$               | 420.4 (M + H) | 3.81                 |
| 3403        | <br><chem>c1ccoc1C(=O)N2CCCC2C3C(=N1)N4C(=N3)NCC4C5=CC=CC=C5N1(C)C</chem><br>$\text{CF}_3\text{CO}_2\text{H}$                    | 381.2 (M + H) | 3.33                 |
| 3404        | <br><chem>CC1=CC=C(C=C1)C(=O)N2CCCC2C3C(=N1)N4C(=N3)NCC4C5=CC=CC=C5N1(C)C</chem><br>$\text{CF}_3\text{CO}_2\text{H}$             | 404.4 (M + H) | 3.93                 |
| 3405        | <br><chem>[O-][N+](=O)c1ccc(cc1)C(=O)N2CCCC2C3C(=N1)N4C(=N3)NCC4C5=CC=CC=C5N1(C)C</chem><br>$\text{CF}_3\text{CO}_2\text{H}$     | 435.2 (M + H) | 3.40                 |
| 3406        | <br><chem>COc1ccc2c(c1)c3c(ccc3N2)C(=O)N4CCCC4C5C(=N1)N6C(=N5)NCC6C7=CC=CC=C7N1(C)C</chem><br>$\text{CF}_3\text{CO}_2\text{H}$ | 484.4 (M + H) | 4.15                 |

| Example No. | Structure   | ESI-MS        | Retention Time (min) |
|-------------|---|---------------|----------------------|
| 3407        | <br>$\text{CF}_3\text{CO}_2\text{H}$   | 469.4 (M + H) | 4.20                 |
| 3408        | <br>$\text{CF}_3\text{CO}_2\text{H}$   | 436.2 (M + H) | 3.88                 |
| 3409        | <br>$\text{CF}_3\text{CO}_2\text{H}$   | 434.4 (M + H) | 3.91                 |
| 3410        | <br>$\text{CF}_3\text{CO}_2\text{H}$   | 558.4 (M + H) | 4.92                 |
| 3411        | <br>$2\text{CF}_3\text{CO}_2\text{H}$  | 483.4 (M + H) | 4.08                 |
| 3412        | <br>$\text{CF}_3\text{CO}_2\text{H}$ | 396.2 (M + H) | 3.68                 |

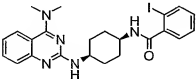
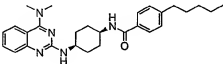
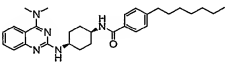
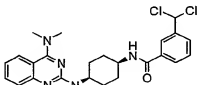
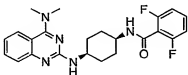
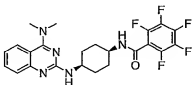
| Example No. | Structure   | ESI-MS        | Retention Time (min) |
|-------------|---|---------------|----------------------|
| 3413        | <br><chem>CC1=C(C)N2C(=N1)N(C)C(=N2)N[C@H]3CCCC[C@H]3NC(=O)COc4ccc(Cl)cc4</chem><br>$\text{CF}_3\text{CO}_2\text{H}$           | 454.2 (M + H) | 3.70                 |
| 3414        | <br><chem>CC1=C(C)N2C(=N1)N(C)C(=N2)N[C@H]3CCCC[C@H]3NC(=O)Cc4ccc(C)cc4[N+](=O)[O-]</chem><br>$\text{CF}_3\text{CO}_2\text{H}$ | 449.4 (M + H) | 4.09                 |
| 3415        | <br><chem>CC1=C(C)N2C(=N1)N(C)C(=N2)N[C@H]3CCCC[C@H]3NC(=O)Cc4cc(F)c(F)c(F)c4</chem><br>$\text{CF}_3\text{CO}_2\text{H}$       | 476.2 (M + H) | 4.33                 |
| 3416        | <br><chem>CC1=C(C)N2C(=N1)N(C)C(=N2)N[C@H]3CCCC[C@H]3NC(=O)Cc4cc(F)c(F)c(F)c4</chem><br>$\text{CF}_3\text{CO}_2\text{H}$       | 476.4 (M + H) | 3.60                 |
| 3417        | <br><chem>CC1=C(C)N2C(=N1)N(C)C(=N2)N[C@H]3CCCC[C@H]3NC(=O)Cc4cc(F)c(F)cc4</chem><br>$\text{CF}_3\text{CO}_2\text{H}$          | 476.4 (M + H) | 4.23                 |
| 3418        | <br><chem>CC1=C(C)N2C(=N1)N(C)C(=N2)N[C@H]3CCCC[C@H]3NC(=O)Cc4cc(F)c(F)c(F)c4</chem><br>$\text{CF}_3\text{CO}_2\text{H}$     | 476.4 (M + H) | 4.38                 |

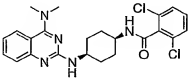
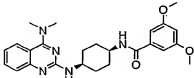
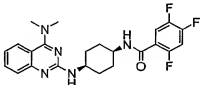
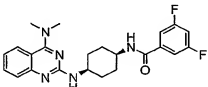
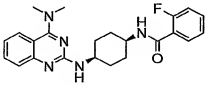
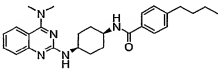


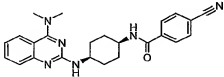
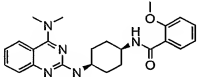
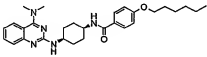
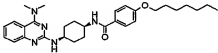
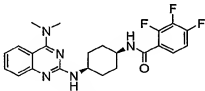
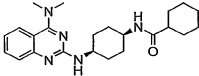
| Example No. | Structure   | ESI-MS        | Retention Time (min) |
|-------------|---|---------------|----------------------|
| 3419        | <br><chem>CC1=NC2=CC=CC=C2N1N[C@H]3CCCC[C@H]3NC(=O)c4cc(F)c(F)cc4</chem><br>$\text{CF}_3\text{CO}_2\text{H}$     | 426.2 (M + H) | 3.87                 |
| 3420        | <br><chem>CC1=NC2=CC=CC=C2N1N[C@H]3CCCC[C@H]3NC(=O)c4cc(F)c(F)c(F)c4</chem><br>$\text{CF}_3\text{CO}_2\text{H}$  | 444.4 (M + H) | 3.86                 |
| 3421        | <br><chem>CC1=NC2=CC=CC=C2N1N[C@H]3CCCC[C@H]3NC(=O)c4cc(F)c(F)c(F)c4F</chem><br>$\text{CF}_3\text{CO}_2\text{H}$ | 462.2 (M + H) | 4.15                 |
| 3422        | <br><chem>CC1=NC2=CC=CC=C2N1N[C@H]3CCCC[C@H]3NC(=O)c4ccc(Cl)cc4</chem><br>$\text{CF}_3\text{CO}_2\text{H}$       | 424.2 (M + H) | 4.06                 |
| 3423        | <br><chem>CC1=NC2=CC=CC=C2N1N[C@H]3CCCC[C@H]3NC(=O)c4cc(OC)c(OC)cc4</chem><br>$\text{CF}_3\text{CO}_2\text{H}$   | 450.4 (M + H) | 4.03                 |
| 3424        | <br><chem>CC1=NC2=CC=CC=C2N1N[C@H]3CCCC[C@H]3NC(=O)c4ccc5c(c4)OCO5</chem><br>$\text{CF}_3\text{CO}_2\text{H}$  | 434.2 (M + H) | 3.75                 |

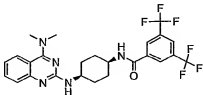
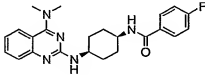
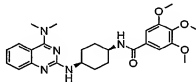
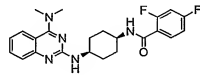
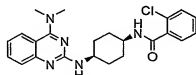
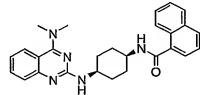
| Example No. | Structure   | ESI-MS        | Retention Time (min) |
|-------------|---|---------------|----------------------|
| 3425        | <br><chem>CC1=NC2=CC=CC=C2N1N[C@H]3CCCC[C@H]3NC(=O)c1cc(F)cc(F)c1</chem><br>$\text{CF}_3\text{CO}_2\text{H}$     | 426.2 (M + H) | 3.88                 |
| 3426        | <br><chem>CC1=NC2=CC=CC=C2N1N[C@H]3CCCC[C@H]3NC(=O)c1cc(OC)c(OC)cc1</chem><br>$\text{CF}_3\text{CO}_2\text{H}$   | 450.4 (M + H) | 3.64                 |
| 3427        | <br><chem>CC1=NC2=CC=CC=C2N1N[C@H]3CCCC[C@H]3NC(=O)c1cc(OC)cc(OC)c1</chem><br>$\text{CF}_3\text{CO}_2\text{H}$   | 450.4 (M + H) | 3.55                 |
| 3428        | <br><chem>CC1=NC2=CC=CC=C2N1N[C@H]3CCCC[C@H]3NC(=O)c1ccc(CC)cc1</chem><br>$\text{CF}_3\text{CO}_2\text{H}$       | 418.6 (M + H) | 4.17                 |
| 3429        | <br><chem>CC1=NC2=CC=CC=C2N1N[C@H]3CCCC[C@H]3NC(=O)c1ccc(OCC)cc1</chem><br>$\text{CF}_3\text{CO}_2\text{H}$      | 434.4 (M + H) | 4.03                 |
| 3430        | <br><chem>CC1=NC2=CC=CC=C2N1N[C@H]3CCCC[C@H]3NC(=O)c1cc(Cl)cc(Cl)c1</chem><br>$\text{CF}_3\text{CO}_2\text{H}$ | 458.2 (M + H) | 4.45                 |

| Example No. | Structure                             | ESI-MS        | Retention Time (min) |
|-------------|---------------------------------------|---------------|----------------------|
| 3431        | <br>CF <sub>3</sub> CO <sub>2</sub> H | 415.4 (M + H) | 3.76                 |
| 3432        | <br>CF <sub>3</sub> CO <sub>2</sub> H | 474.4 (M + H) | 5.06                 |
| 3433        | <br>CF <sub>3</sub> CO <sub>2</sub> H | 410.2 (M + H) | 3.64                 |
| 3434        | <br>CF <sub>3</sub> CO <sub>2</sub> H | 516.2 (M + H) | 4.24                 |
| 3435        | <br>CF <sub>3</sub> CO <sub>2</sub> H | 424.2 (M + H) | 4.09                 |
| 3436        | <br>CF <sub>3</sub> CO <sub>2</sub> H | 458.2 (M + H) | 3.89                 |

| Example No. | Structure   | ESI-MS        | Retention Time (min) |
|-------------|---|---------------|----------------------|
| 3437        | <br>$\text{CF}_3\text{CO}_2\text{H}$   | 516.2 (M + H) | 3.88                 |
| 3438        | <br>$\text{CF}_3\text{CO}_2\text{H}$   | 460.4 (M + H) | 4.86                 |
| 3439        | <br>$\text{CF}_3\text{CO}_2\text{H}$   | 488.4 (M + H) | 4.70                 |
| 3440        | <br>$\text{CF}_3\text{CO}_2\text{H}$   | 472.4 (M + H) | 4.29                 |
| 3441        | <br>$\text{CF}_3\text{CO}_2\text{H}$   | 426.2 (M + H) | 3.69                 |
| 3442        | <br>$\text{CF}_3\text{CO}_2\text{H}$ | 480.2 (M + H) | 4.16                 |

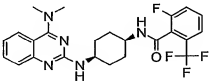
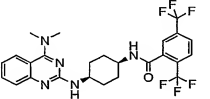
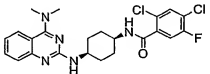
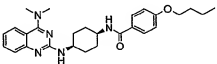
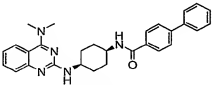
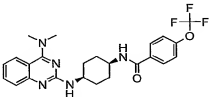
| Example No. | Structure   | ESI-MS        | Retention Time (min) |
|-------------|---|---------------|----------------------|
| 3443        | <br>$\text{CF}_3\text{CO}_2\text{H}$   | 458.2 (M + H) | 3.91                 |
| 3444        | <br>$\text{CF}_3\text{CO}_2\text{H}$   | 450.4 (M + H) | 3.95                 |
| 3445        | <br>$\text{CF}_3\text{CO}_2\text{H}$   | 444.4 (M + H) | 4.01                 |
| 3446        | <br>$\text{CF}_3\text{CO}_2\text{H}$   | 426.2 (M + H) | 4.00                 |
| 3447        | <br>$\text{CF}_3\text{CO}_2\text{H}$   | 408.4 (M + H) | 3.75                 |
| 3448        | <br>$\text{CF}_3\text{CO}_2\text{H}$ | 446.6 (M + H) | 4.65                 |

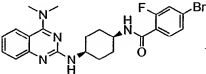
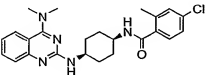
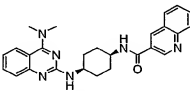
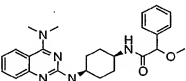
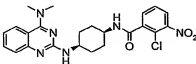
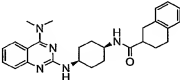
| Example No. | Structure   | ESI-MS        | Retention Time (min) |
|-------------|---|---------------|----------------------|
| 3449        | <br><chem>CC1=NC2=CC=CC=C2N(C)N1C3=CC=CC=C3N3C(=O)C4=CC=C(C#N)C=C4</chem><br>$\text{CF}_3\text{CO}_2\text{H}$          | 415.2 (M + H) | 3.75                 |
| 3450        | <br><chem>COc1ccc(cc1)C(=O)N[C@H]2CCCC[C@H]2c3nc4c(ncn4C)C5=CC=CC=C5N3C</chem><br>$\text{CF}_3\text{CO}_2\text{H}$     | 420.4 (M + H) | 3.91                 |
| 3451        | <br><chem>CCOC1=CC=C(C=C1)C(=O)N[C@H]2CCCC[C@H]2c3nc4c(ncn4C)C5=CC=CC=C5N3C</chem><br>$\text{CF}_3\text{CO}_2\text{H}$ | 490.4 (M + H) | 4.99                 |
| 3452        | <br><chem>CCOC1=CC=C(C=C1)C(=O)N[C@H]2CCCC[C@H]2c3nc4c(ncn4C)C5=CC=CC=C5N3C</chem><br>$\text{CF}_3\text{CO}_2\text{H}$ | 504.4 (M + H) | 5.16                 |
| 3453        | <br><chem>Fc1cc(F)c(cc1)C(=O)N[C@H]2CCCC[C@H]2c3nc4c(ncn4C)C5=CC=CC=C5N3C</chem><br>$\text{CF}_3\text{CO}_2\text{H}$   | 444.4 (M + H) | 4.00                 |
| 3454        | <br><chem>C1CCCCC1C(=O)N[C@H]2CCCC[C@H]2c3nc4c(ncn4C)C5=CC=CC=C5N3C</chem><br>$\text{CF}_3\text{CO}_2\text{H}$       | 396.2 (M + H) | 3.85                 |

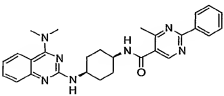
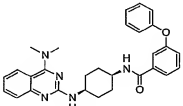
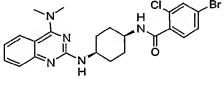
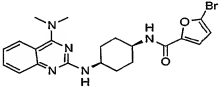
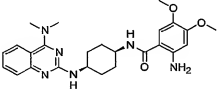
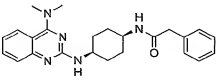
| Example No. | Structure   | ESI-MS        | Retention Time (min) |
|-------------|---|---------------|----------------------|
| 3455        | <br>$\text{CF}_3\text{CO}_2\text{H}$   | 526.6 (M + H) | 4.69                 |
| 3456        | <br>$\text{CF}_3\text{CO}_2\text{H}$   | 408.4 (M + H) | 3.30                 |
| 3457        | <br>$\text{CF}_3\text{CO}_2\text{H}$   | 480.4 (M + H) | 3.76                 |
| 3458        | <br>$\text{CF}_3\text{CO}_2\text{H}$   | 426.2 (M + H) | 3.86                 |
| 3459        | <br>$\text{CF}_3\text{CO}_2\text{H}$   | 424.2 (M + H) | 3.76                 |
| 3460        | <br>$\text{CF}_3\text{CO}_2\text{H}$ | 440.4 (M + H) | 4.05                 |

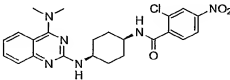
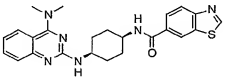
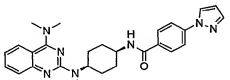
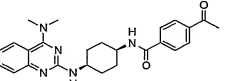
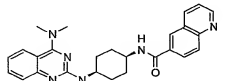
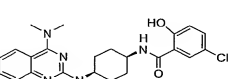




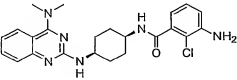
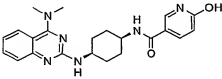
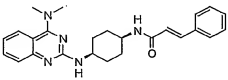
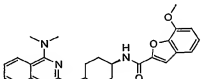
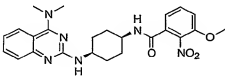
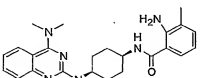
| Example No. | Structure   | ESI-MS        | Retention Time (min) |
|-------------|---|---------------|----------------------|
| 3467        | <br>$\text{CF}_3\text{CO}_2\text{H}$   | 476.2 (M + H) | 3.92                 |
| 3468        | <br>$\text{CF}_3\text{CO}_2\text{H}$   | 526.4 (M + H) | 4.31                 |
| 3469        | <br>$\text{CF}_3\text{CO}_2\text{H}$   | 476.2 (M + H) | 4.15                 |
| 3470        | <br>$\text{CF}_3\text{CO}_2\text{H}$   | 462.2 (M + H) | 4.48                 |
| 3471        | <br>$\text{CF}_3\text{CO}_2\text{H}$   | 466.4 (M + H) | 4.45                 |
| 3472        | <br>$\text{CF}_3\text{CO}_2\text{H}$ | 474.4 (M + H) | 4.29                 |

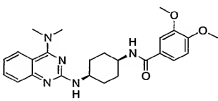
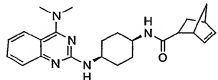
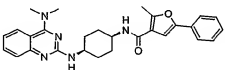
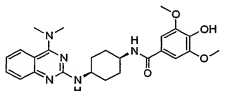
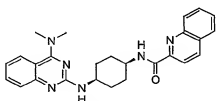
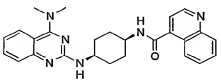
| Example No. | Structure   | ESI-MS        | Retention Time (min) |
|-------------|---|---------------|----------------------|
| 3473        | <br>$\text{CF}_3\text{CO}_2\text{H}$   | 486.2 (M + H) | 4.32                 |
| 3474        | <br>$\text{CF}_3\text{CO}_2\text{H}$   | 438.4 (M + H) | 4.31                 |
| 3475        | <br>$2\text{CF}_3\text{CO}_2\text{H}$  | 441.4 (M + H) | 3.75                 |
| 3476        | <br>$\text{CF}_3\text{CO}_2\text{H}$   | 434.4 (M + H) | 4.10                 |
| 3477        | <br>$\text{CF}_3\text{CO}_2\text{H}$   | 469.4 (M + H) | 4.19                 |
| 3478        | <br>$\text{CF}_3\text{CO}_2\text{H}$ | 444.4 (M + H) | 4.36                 |

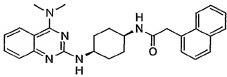
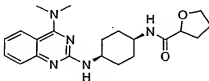
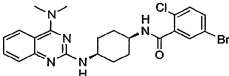
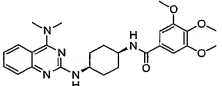
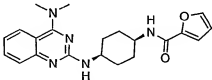
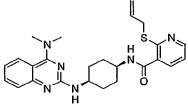
| Example No. | Structure  | ESI-MS        | Retention Time (min) |
|-------------|--|---------------|----------------------|
| 3479        |  <p>3CF<sub>3</sub>CO<sub>2</sub>H</p>  | 482.4 (M + H) | 4.35                 |
| 3480        |  <p>CF<sub>3</sub>CO<sub>2</sub>H</p>   | 482.4 (M + H) | 4.64                 |
| 3481        |  <p>CF<sub>3</sub>CO<sub>2</sub>H</p>   | 502.2 (M + H) | 4.37                 |
| 3482        |  <p>CF<sub>3</sub>CO<sub>2</sub>H</p>   | 458.2 (M + H) | 4.08                 |
| 3483        |  <p>2CF<sub>3</sub>CO<sub>2</sub>H</p>  | 465.4 (M + H) | 3.66                 |
| 3484        |  <p>CF<sub>3</sub>CO<sub>2</sub>H</p> | 404.4 (M + H) | 4.03                 |

| Example No. | Structure   | ESI-MS        | Retention Time (min) |
|-------------|---|---------------|----------------------|
| 3485        | <br>$\text{CF}_3\text{CO}_2\text{H}$   | 469.4 (M + H) | 4.23                 |
| 3486        | <br>$2\text{CF}_3\text{CO}_2\text{H}$  | 447.4 (M + H) | 3.94                 |
| 3487        | <br>$2\text{CF}_3\text{CO}_2\text{H}$  | 456.2 (M + H) | 4.07                 |
| 3488        | <br>$\text{CF}_3\text{CO}_2\text{H}$   | 432.4 (M + H) | 3.99                 |
| 3489        | <br>$2\text{CF}_3\text{CO}_2\text{H}$  | 441.3 (M + H) | 1.70                 |
| 3490        | <br>$\text{CF}_3\text{CO}_2\text{H}$ | 440.2 (M + H) | 4.57                 |

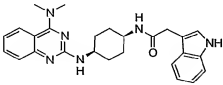
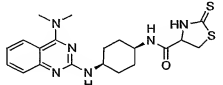
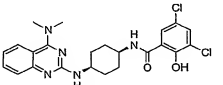
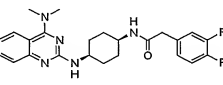
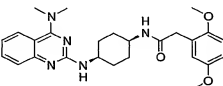
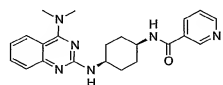


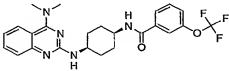
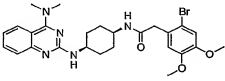
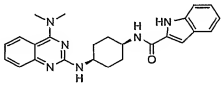
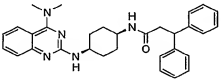
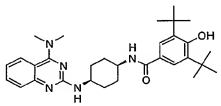
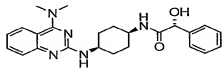
| Example No. | Structure  | ESI-MS        | Retention Time (min) |
|-------------|--|---------------|----------------------|
| 3497        | <br>$2\text{CF}_3\text{CO}_2\text{H}$   | 439.4 (M + H) | 1.93                 |
| 3498        | <br>$2\text{CF}_3\text{CO}_2\text{H}$   | 407.4 (M + H) | 1.62                 |
| 3499        | <br>$\text{CF}_3\text{CO}_2\text{H}$    | 416.3 (M + H) | 2.34                 |
| 3500        | <br>$\text{CF}_3\text{CO}_2\text{H}$    | 460.4 (M + H) | 2.46                 |
| 3501        | <br>$\text{CF}_3\text{CO}_2\text{H}$    | 465.4 (M + H) | 4.13                 |
| 3502        | <br>$2\text{CF}_3\text{CO}_2\text{H}$ | 419.4 (M + H) | 3.87                 |

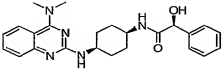
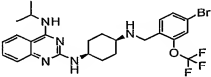
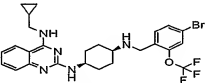
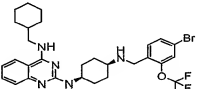
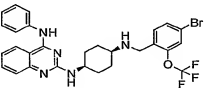
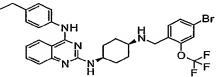
| Example No. | Structure  | ESI-MS        | Retention Time (min) |
|-------------|--|---------------|----------------------|
| 3503        | <br>$\text{CF}_3\text{CO}_2\text{H}$    | 450.4 (M + H) | 3.97                 |
| 3504        | <br>$\text{CF}_3\text{CO}_2\text{H}$    | 406.2 (M + H) | 2.18                 |
| 3505        | <br>$\text{CF}_3\text{CO}_2\text{H}$    | 470.4 (M + H) | 4.74                 |
| 3506        | <br>$\text{CF}_3\text{CO}_2\text{H}$    | 466.4 (M + H) | 3.83                 |
| 3507        | <br>$2\text{CF}_3\text{CO}_2\text{H}$   | 441.2 (M + H) | 4.38                 |
| 3508        | <br>$2\text{CF}_3\text{CO}_2\text{H}$ | 441.2 (M + H) | 3.62                 |

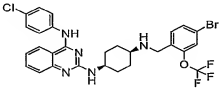
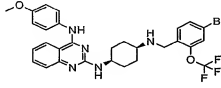
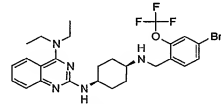
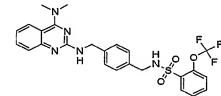
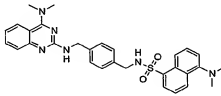
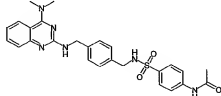
| Example No. | Structure  | ESI-MS        | Retention Time (min) |
|-------------|--|---------------|----------------------|
| 3509        | <br>$\text{CF}_3\text{CO}_2\text{H}$    | 454.5 (M + H) | 2.44                 |
| 3510        | <br>$\text{CF}_3\text{CO}_2\text{H}$    | 384.4 (M + H) | 3.67                 |
| 3511        | <br>$\text{CF}_3\text{CO}_2\text{H}$    | 502.2 (M + H) | 4.37                 |
| 3512        | <br>$\text{CF}_3\text{CO}_2\text{H}$    | 480.5 (M + H) | 2.18                 |
| 3513        | <br>$\text{CF}_3\text{CO}_2\text{H}$    | 380.2 (M + H) | 3.81                 |
| 3514        | <br>$2\text{CF}_3\text{CO}_2\text{H}$ | 463.2 (M + H) | 4.23                 |

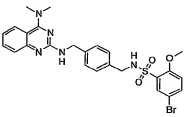
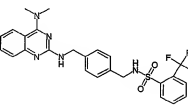
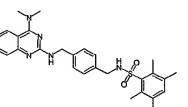
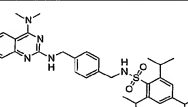
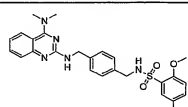
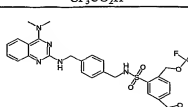


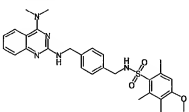
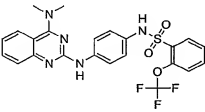
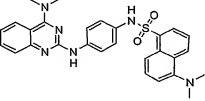
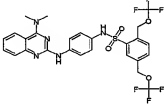
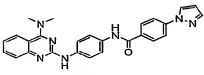
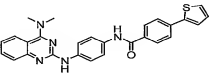
| Example No. | Structure   | ESI-MS        | Retention Time (min) |
|-------------|---|---------------|----------------------|
| 3515        | <br><chem>CC1(C)N2C(=NC3=CC=CC=C3N2)N(C1)C(=O)NCC4=CC=C5C(=C4)N=CN=C5</chem><br>$2\text{CF}_3\text{CO}_2\text{H}$  | 443.4 (M + H) | 2.12                 |
| 3516        | <br><chem>CC1(C)N2C(=NC3=CC=CC=C3N2)N(C1)C(=O)NCC4=NN=C(S4)</chem><br>$\text{CF}_3\text{CO}_2\text{H}$             | 431.1 (M + H) | 1.90                 |
| 3517        | <br><chem>CC1(C)N2C(=NC3=CC=CC=C3N2)N(C1)C(=O)NCC4=CC(=C(C=C4)Cl)C(=O)O</chem><br>$\text{CF}_3\text{CO}_2\text{H}$ | 474.4 (M + H) | 5.05                 |
| 3518        | <br><chem>CC1(C)N2C(=NC3=CC=CC=C3N2)N(C1)C(=O)NCC4=CC(=C(C=C4)F)C(=O)F</chem><br>$\text{CF}_3\text{CO}_2\text{H}$  | 440.5 (M + H) | 2.33                 |
| 3519        | <br><chem>CC1(C)N2C(=NC3=CC=CC=C3N2)N(C1)C(=O)NCC4=CC(=C(C=C4)OC)OC</chem><br>$\text{CF}_3\text{CO}_2\text{H}$     | 464.5 (M + H) | 2.20                 |
| 3520        | <br><chem>CC1(C)N2C(=NC3=CC=CC=C3N2)N(C1)C(=O)NCC4=CC=CC=N4</chem><br>$2\text{CF}_3\text{CO}_2\text{H}$          | 391.1 (M + H) | 1.59                 |

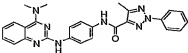
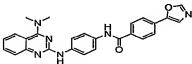
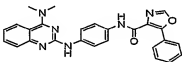
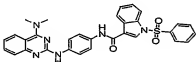
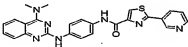
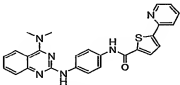
| Example No. | Structure   | ESI-MS        | Retention Time (min) |
|-------------|---|---------------|----------------------|
| 3521        | <br>$\text{CF}_3\text{CO}_2\text{H}$   | 474.4 (M + H) | 4.53                 |
| 3522        | <br>$\text{CF}_3\text{CO}_2\text{H}$   | 542.2 (M + H) | 2.26                 |
| 3523        | <br>$2\text{CF}_3\text{CO}_2\text{H}$  | 429.3 (M + H) | 2.41                 |
| 3524        | <br>$\text{CF}_3\text{CO}_2\text{H}$   | 494.6 (M + H) | 2.59                 |
| 3525        | <br>$\text{CF}_3\text{CO}_2\text{H}$   | 518.5 (M + H) | 2.96                 |
| 3526        | <br>$\text{CF}_3\text{CO}_2\text{H}$ | 420.4 (M + H) | 2.19                 |

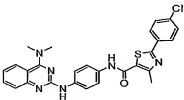
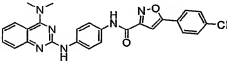
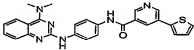
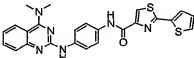
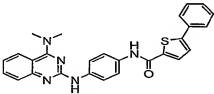
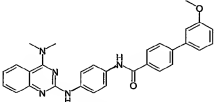
| Example No. | Structure   | ESI-MS        | Retention Time (min) |
|-------------|---|---------------|----------------------|
| 3527        | <br><chem>CC1(C)N2C(=NC3C(=N2)N(C)C3)NC(=O)C1Cc1ccccc1O</chem><br>$\text{CF}_3\text{CO}_2\text{H}$                         | 420.4 (M + H) | 2.19                 |
| 3528        | <br><chem>CC(C)N1C2C(=NC3C(=N2)N(C)C3)NC(=O)C1Cc1ccc(Br)c(OC(F)(F)F)c1</chem><br>$2\text{CF}_3\text{CO}_2\text{H}$         | 552.0 (M + H) | 2.45                 |
| 3529        | <br><chem>C1CC1N2C(=NC3C(=N2)N(C)C3)NC(=O)C2Cc1ccc(Br)c(OC(F)(F)F)c1</chem><br>$2\text{CF}_3\text{CO}_2\text{H}$           | 564.2 (M + H) | 2.48                 |
| 3530        | <br><chem>C1CCCCC1CN2C(=NC3C(=N2)N(C)C3)NC(=O)C1Cc1ccc(Br)c(OC(F)(F)F)c1</chem><br>$2\text{CF}_3\text{CO}_2\text{H}$       | 606.0 (M + H) | 2.86                 |
| 3531        | <br><chem>c1ccc(NC2C(=NC3C(=N2)N(C)C3)NC(=O)C2Cc1ccc(Br)c(OC(F)(F)F)c1)cc1</chem><br>$2\text{CF}_3\text{CO}_2\text{H}$     | 586.2 (M + H) | 3.20                 |
| 3532        | <br><chem>CCc1ccc(NC2C(=NC3C(=N2)N(C)C3)NC(=O)C2Cc1ccc(Br)c(OC(F)(F)F)c1)cc1</chem><br>$2\text{CF}_3\text{CO}_2\text{H}$ | 614.4 (M + H) | 2.76                 |

| Example No. | Structure   | ESI-MS        | Retention Time (min) |
|-------------|---|---------------|----------------------|
| 3533        | <br>$2\text{CF}_3\text{CO}_2\text{H}$  | 620.0 (M + H) | 2.68                 |
| 3534        | <br>$2\text{CF}_3\text{CO}_2\text{H}$  | 616.0 (M + H) | 2.56                 |
| 3535        | <br>$2\text{CF}_3\text{CO}_2\text{H}$  | 566.0 (M + H) | 2.54                 |
| 3536        | <br>$\text{CF}_3\text{CO}_2\text{H}$   | 532.2 (M + H) | 3.35                 |
| 3537        | <br>$2\text{CF}_3\text{CO}_2\text{H}$  | 541.4 (M + H) | 3.11                 |
| 3538        | <br>$\text{CF}_3\text{CO}_2\text{H}$ | 505.2 (M + H) | 2.98                 |

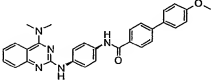
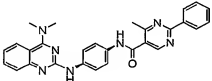
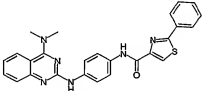
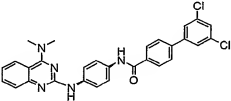
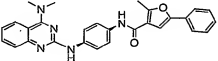
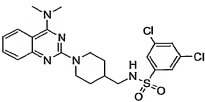
| Example No. | Structure   | ESI-MS        | Retention Time (min) |
|-------------|---|---------------|----------------------|
| 3539        | <br><chem>CC1=NC2=CC=CC=C2N=CN=C1NCCc3ccc(cc3)CNS(=O)(=O)c4cc(OC)cc(Br)c4</chem><br>$\text{CF}_3\text{CO}_2\text{H}$       | 556 (M + H)   | 3.37                 |
| 3540        | <br><chem>CC1=NC2=CC=CC=C2N=CN=C1NCCc3ccc(cc3)CNS(=O)(=O)c4cc(F)(F)Fcc4</chem><br>$\text{CF}_3\text{CO}_2\text{H}$         | 516.4 (M + H) | 3.39                 |
| 3541        | <br><chem>CC1=NC2=CC=CC=C2N=CN=C1NCCc3ccc(cc3)CNS(=O)(=O)c4cc(C)c(C)c(C)c4</chem><br>$\text{CF}_3\text{CO}_2\text{H}$      | 504.4 (M + H) | 3.61                 |
| 3542        | <br><chem>CC1=NC2=CC=CC=C2N=CN=C1NCCc3ccc(cc3)CNS(=O)(=O)c4cc(C)c(C)c(C)c4</chem><br>$\text{CF}_3\text{CO}_2\text{H}$      | 574.4 (M + H) | 4.27                 |
| 3543        | <br><chem>CC1=NC2=CC=CC=C2N=CN=C1NCCc3ccc(cc3)CNS(=O)(=O)c4cc(OC)cc(Cl)c4</chem><br>$\text{CF}_3\text{CO}_2\text{H}$       | 508.2 (M + H) | 3.17                 |
| 3544        | <br><chem>CC1=NC2=CC=CC=C2N=CN=C1NCCc3ccc(cc3)CNS(=O)(=O)c4ccc(cc4)COC(F)(F)F</chem><br>$\text{CF}_3\text{CO}_2\text{H}$ | 644.2 (M + H) | 3.63                 |

| Example No. | Structure   | ESI-MS        | Retention Time (min) |
|-------------|---|---------------|----------------------|
| 3545        | <br>$\text{CF}_3\text{CO}_2\text{H}$   | 520.4 (M + H) | 3.56                 |
| 3546        | <br>$\text{CF}_3\text{CO}_2\text{H}$   | 504.2 (M + H) | 3.25                 |
| 3547        | <br>$2\text{CF}_3\text{CO}_2\text{H}$  | 513.4 (M + H) | 2.86                 |
| 3548        | <br>$\text{CF}_3\text{CO}_2\text{H}$   | 616.2 (M + H) | 3.73                 |
| 3549        | <br>$2\text{CF}_3\text{CO}_2\text{H}$  | 450.4 (M + H) | 2.79                 |
| 3550        | <br>$\text{CF}_3\text{CO}_2\text{H}$ | 466.2 (M + H) | 3.35                 |

| Example No. | Structure  | ESI-MS        | Retention Time (min) |
|-------------|--|---------------|----------------------|
| 3551        | <br>$2\text{CF}_3\text{CO}_2\text{H}$   | 465.2 (M + H) | 3.34                 |
| 3552        | <br>$\text{CF}_3\text{CO}_2\text{H}$    | 451.2 (M + H) | 3.83                 |
| 3553        | <br>$\text{CF}_3\text{CO}_2\text{H}$    | 451.2 (M + H) | 4.10                 |
| 3554        | <br>$\text{CF}_3\text{CO}_2\text{H}$    | 563.2 (M + H) | 4.33                 |
| 3555        | <br>$2\text{CF}_3\text{CO}_2\text{H}$   | 468.4 (M + H) | 3.66                 |
| 3556        | <br>$2\text{CF}_3\text{CO}_2\text{H}$ | 467.4 (M + H) | 2.85                 |

| Example No. | Structure   | ESI-MS        | Retention Time (min) |
|-------------|---|---------------|----------------------|
| 3557        | <br>$\text{CF}_3\text{CO}_2\text{H}$   | 515.4 (M + H) | 3.52                 |
| 3558        | <br>$\text{CF}_3\text{CO}_2\text{H}$   | 485.2 (M + H) | 3.40                 |
| 3559        | <br>$2\text{CF}_3\text{CO}_2\text{H}$  | 467.4 (M + H) | 3.90                 |
| 3560        | <br>$\text{CF}_3\text{CO}_2\text{H}$   | 473.4 (M + H) | 4.17                 |
| 3561        | <br>$\text{CF}_3\text{CO}_2\text{H}$   | 467.4 (M + H) | 3.57                 |
| 3562        | <br>$\text{CF}_3\text{CO}_2\text{H}$ | 490.2 (M + H) | 4.00                 |



| Example No. | Structure  | ESI-MS        | Retention Time (min) |
|-------------|--|---------------|----------------------|
| 3563        | <br><chem>CN1C=NC2=C(N1)N=CN=C2c3ccc(NC(=O)c4ccc(OC)cc4)cc3</chem><br>$\text{CF}_3\text{CO}_2\text{H}$            | 490.2 (M + H) | 3.99                 |
| 3564        | <br><chem>CN1C=NC2=C(N1)N=CN=C2c3ccc(NC(=O)c4nc(C5=CC=CC=C5)nnc45)cc3</chem><br>$2\text{CF}_3\text{CO}_2\text{H}$ | 476.2 (M + H) | 3.76                 |
| 3565        | <br><chem>CN1C=NC2=C(N1)N=CN=C2c3ccc(NC(=O)c4nnsc45)cc3</chem><br>$\text{CF}_3\text{CO}_2\text{H}$                | 467.2 (M + H) | 4.07                 |
| 3566        | <br><chem>CN1C=NC2=C(N1)N=CN=C2c3ccc(NC(=O)c4cc(Cl)cc(Cl)c4)cc3</chem><br>$\text{CF}_3\text{CO}_2\text{H}$        | 528.2 (M + H) | 4.53                 |
| 3567        | <br><chem>CN1C=NC2=C(N1)N=CN=C2c3ccc(NC(=O)c4oc(C5=CC=CC=C5)cc45)cc3</chem><br>$\text{CF}_3\text{CO}_2\text{H}$   | 464.2 (M + H) | 4.11                 |
| 3568        | <br><chem>CN1C=NC2=C(N1)N=CN=C2c3ccc(S(=O)(=O)c4cc(Cl)cc(Cl)c4)cc3</chem><br>$\text{CF}_3\text{CO}_2\text{H}$   | 494.0 (M + H) | 3.43                 |





## Assay Procedures

Compounds identified and disclosed throughout this patent document were assayed according to the protocols found in co-pending patent application having U.S. Serial Number 09/826,509, which is incorporated herein by reference.

### Example 3580

#### Preparation of Endogenous MCH Receptor.

The endogenous human MCH receptor was obtained by PCR using genomic DNA as template and rTth polymerase (Perkin Elmer) with the buffer system provided by the manufacturer, 0.25  $\mu$ M of each primer, and 0.2 mM of each 4 nucleotides. The cycle condition was 30 cycles of 94°C for 1 min, 56°C for 1min and 72 °C for 1 min and 20 sec. The 5' PCR primer contained a HindIII site with the sequence:

5'-GTGAAGCTTGCCTCTGGTGCCTGCAGGAGG-3' (SEQ.ID.NO.:1)

and the 3' primer contained an EcoRI site with the sequence:

5'-GCAGAATCCCGTGGCGTGTGTGGTGCCC-3' (SEQ.ID.NO.:2).

The 1.3 kb PCR fragment was digested with HindIII and EcoRI and cloned into HindIII-EcoRI site of CMVp expression vector. Later the cloning work by Lakaye et al showed that there is an intron in the coding region of the gene. Thus the 5' end of the cDNA was obtained by 5' RACE PCR using Clontech's marathon-ready hypothalamus cDNA as template and the manufacturer's recommended protocol for cycling condition. The 5' RACE PCR for the first and second round PCR were as follows:

5'-CATGAGCTGGTGGATCATGAAGGG-3' (SEQ.ID.NO.:3) and

5'-ATGAAGGGCATGCCAGGAGAAAG-3' (SEQ.ID.NO.:4).

Nucleic acid and amino acid sequences were thereafter determined and verified with the published sequences found on GenBank having Accession Number U71092.

### Example 3581

#### Preparation of Non-Endogenous, Constitutively Active MCH Receptor.

Preparation of a non-endogenous version of the human MCH receptor was accomplished by creating a MCH-IC3-SST2 mutation (*see*; SEQ.ID.NO.:7 for nucleic acid sequence, and SEQ.ID.NO.:8 for amino acid sequence). Blast result showed that MCH receptor had the highest sequence homology to known SST2 receptor. Thus the third intracellular loop ("IC3") of MCH receptor was replaced with that of the IC3 of SST2

receptor to see if the chimera would show constitutive activity.

The BamHI-BstEII fragment containing IC3 of MCH receptor was replaced with synthetic oligonucleotides that contained the IC3 of SST2. The PCR sense mutagenesis primer used had the following sequence:

5'-GATCCTGCAGAAGGTGAAGTCTCTGGAATCCGAGTGGGCTCCTCTAAGAG  
GAAGAAGTCTGAGAAGAAG-3' (SEQ.ID.NO.:9)

and the antisense primer had the following sequence:

5'-GTGACCTTCTTCTCAGACTTCTTCTCTTAGAGGAGCCCACTCGGATTCCAG  
AGGACTTCACCTTCTGCAG-3' (SEQ.ID.NO.:10).

The endogenous MCH receptor cDNA was used as a template.

### Example 3582

#### GPCR Fusion Protein Preparation.

MCH Receptor-Gi $\alpha$  Fusion Protein construct was made as follows: primers were designed for endogenous MCH receptor was as follows:

5'-GTGAAGCTTGCCCGGGCAGGATGGACCTGG-3' (SEQ.ID.NO.:11; sense)

5'-ATCTAGAGGTGCCTTTGCTTTCTG-3' (SEQ.ID.NO.:12; antisense).

The sense and anti-sense primers included the restriction sites for KB4 and XbaI, respectively.

PCR was utilized to secure the respective receptor sequences for fusion within the Gi $\alpha$  universal vector disclosed above, using the following protocol for each: 100ng cDNA for MCH receptor was added to separate tubes containing 2ul of each primer (sense and anti-sense), 3uL of 10mM dNTPs, 10uL of 10XTaqPlus™ Precision buffer, 1uL of TaqPlus™ Precision polymerase (Stratagene: #600211), and 80uL of water. Reaction temperatures and cycle times for MCH receptor were as follows: the initial denaturing step was done at 94°C for five minutes, and a cycle of 94°C for 30 seconds; 55°C for 30 seconds; 72°C for two minutes. A final extension time was done at 72°C for ten minutes. PCR product was run on a 1% agarose gel and then purified (data not shown). The purified product was digested with KB4 and XbaI (New England Biolabs) and the desired inserts will be isolated, purified and ligated into the Gi universal vector at the respective restriction site. The positive clones were isolated following transformation and determined by restriction enzyme digest; expression using 293 cells was accomplished

following the protocol set forth *infra*. Each positive clone for MCH receptor: Gi-Fusion Protein was sequenced and made available for the direct identification of candidate compounds. (See, SEQ.ID.NO.:13 for nucleic acid sequence and SEQ.ID.NO.:14 for amino acid sequence).

Endogenous version of MCH receptor was fused upstream from the G protein Gi and is located at nucleotide 1 through 1,059 (see, SEQ.ID.NO.:13) and amino acid residue 1 through 353 (see, SEQ.ID.NO.:14). With respect to the MCH receptor, 2 amino acid residues (an equivalent of 6 nucleotides) were placed in between the endogenous (or non-endogenous) GPCR and the start codon for the G protein  $G_{i\alpha}$ . Therefore, the Gi protein is located at nucleotide 1,066 through 2,133 (see, SEQ.ID.NO.:13) and at amino acid residue 356 through 711 (see, SEQ.ID.NO.:14). Those skilled in the art are credited with the ability to select techniques for constructing a GPCR Fusion Protein where the G protein is fused to the 3' end of the GPCR of interest.

### Example 3583

#### ASSAY FOR DETERMINATION OF CONSTITUTIVE ACTIVITY OF NON- ENDOGENOUS GPCRS

##### A. Intracellular $IP_3$ Accumulation Assay

On day 1, cells comprising the receptors (endogenous and/or non-endogenous) can be plated onto 24 well plates, usually  $1 \times 10^5$  cells/well (although this number can be optimized). On day 2 cells can be transfected by firstly mixing 0.25  $\mu$ g DNA in 50  $\mu$ l serum free DMEM/well and 2  $\mu$ l lipofectamine in 50  $\mu$ l serum-free DMEM/well. The solutions are gently mixed and incubated for 15-30 min at room temperature. Cells are washed with 0.5 ml PBS and 400  $\mu$ l of serum free media is mixed with the transfection media and added to the cells. The cells are then incubated for 3-4 hrs at 37°C/5%CO<sub>2</sub> and then the transfection media is removed and replaced with 1ml/well of regular growth media. On day 3 the cells are labeled with <sup>3</sup>H-myo-inositol. Briefly, the media is removed and the cells are washed with 0.5 ml PBS. Then 0.5 ml inositol-free/serum free media (GIBCO BRL) is added/well with 0.25  $\mu$ Ci of <sup>3</sup>H-myo-inositol/well and the cells are incubated for 16-18 hrs o/n at 37°C/5%CO<sub>2</sub>. On Day 4 the cells are washed with 0.5 ml PBS and 0.45 ml of assay medium is added containing inositol-free/serum free media 10  $\mu$ M pargyline 10 mM lithium chloride or 0.4 ml of assay medium and 50  $\mu$ l of 10x

ketanserin (ket) to final concentration of 10 $\mu$ M. The cells are then incubated for 30 min at 37°C. The cells are then washed with 0.5 ml PBS and 200  $\mu$ l of fresh/ice cold stop solution (1M KOH; 18 mM Na-borate; 3.8 mM EDTA) is added/well. The solution is kept on ice for 5-10 min or until cells were lysed and then neutralized by 200  $\mu$ l of fresh/ice cold neutralization sol. (7.5 % HCL). The lysate is then transferred into 1.5 ml eppendorf tubes and 1 ml of chloroform/methanol (1:2) is added/tube. The solution is vortexed for 15 sec and the upper phase is applied to a Biorad AG1-X8™ anion exchange resin (100-200 mesh). Firstly, the resin is washed with water at 1:1.25 W/V and 0.9 ml of upper phase is loaded onto the column. The column is washed with 10 mls of 5 mM myo-inositol and 10 ml of 5 mM Na-borate/60mM Na-formate. The inositol tris phosphates are eluted into scintillation vials containing 10 ml of scintillation cocktail with 2 ml of 0.1 M formic acid/ 1 M ammonium formate. The columns are regenerated by washing with 10 ml of 0.1 M formic acid/3M ammonium formate and rinsed twice with H<sub>2</sub>O and stored at 4°C in water.

Reference is made to Figure 1. Figure 1 provides an illustration of IP<sub>3</sub> production from several non-endogenous, constitutively activated version of MCH receptor as compared with the endogenous version of this receptor. When compared to the endogenous version of MCH receptor ("MCH-R wt"), MCH-IC3-SST2 evidenced about a 27% increase in IP<sub>3</sub> accumulation.

#### **Example 3584**

##### **Determination of Compound Using [<sup>35</sup>S]GTP $\gamma$ S ASSAY**

Direct identification of candidate compounds was initially screened using [<sup>35</sup>S]GTP $\gamma$ S Assay (see, Example 6 of co-pending patent application 09/826,509). Preferably, an MCH receptor: Gi Fusion Protein was utilized, according to Example 6(2) of co-pending patent application 09/826,509. Several lead hits were identified utilizing [<sup>35</sup>S]GTP $\gamma$ S Assay.

#### **Example 3585**

##### **High Throughput Functional Screening: FLIPR™**

Subsequently, a functional based assay was used to confirm the lead hits, referred to as FLIPR™ (the Fluorometric Imaging Plate Reader) and FDSS6000™ (Functional

Drug Screening System). This assay utilized a non-endogenous version of the MCH receptor, which was created by swapping the third intracellular loop of the MCH receptor with that of the SST2 receptor (see Example 2(B)(2) of patent application serial number 09/826,509).

The FLIPR and FDSS assays are able to detect intracellular  $\text{Ca}^{2+}$  concentration in cells, which can be utilized to assess receptor activation and determine whether a candidate compound is an, for example, antagonist, inverse agonist or agonist to a Gq-coupled receptor. The concentration of free  $\text{Ca}^{2+}$  in the cytosol of any cell is extremely low, whereas its concentration in the extracellular fluid and endoplasmic reticulum (ER) is very high. Thus, there is a large gradient tending to drive  $\text{Ca}^{2+}$  into the cytosol across both the plasma membrane and ER. The FLIPR<sup>TM</sup> and FDSS6000<sup>TM</sup> systems (Molecular Devices Corporation, HAMAMATSU Photonics K.K.) are designed to perform functional cell-based assays, such as the measurement of intracellular calcium for high-throughput screening. The measurement of fluorescent is associated with calcium release upon activation of the Gq-coupled receptors. Gi or Go coupled receptors are not as easily monitored through the FLIPR<sup>TM</sup> and FDSS6000<sup>TM</sup> systems because these G proteins do not couple with calcium signal pathways.

To confirm the lead hits identified using the [<sup>35</sup>S]GTPγS assay, Fluorometric Imaging Plate Reader system was used to allow for rapid, kinetic measurements of intracellular fluorescence in 96 well microplates (or 384 well microplates). Simultaneous measurements of fluorescence in all wells can be made by FLIPR or FDSS6000<sup>TM</sup> every second with high sensitivity and precision. These systems are ideal for measuring cell-based functional assays such as monitoring the intracellular calcium fluxes that occur within seconds after activation of the Gq coupled receptor.

Briefly, the cells are seeded into 96 well at  $5.5 \times 10^4$  cells/well with complete culture media (Dulbecco's Modified Eagle Medium with 10 % fetal bovine serum, 2 mM L-glutamine, 1 mM sodium pyruvate and 0.5 mg/ml G418, pH 7.4) for the assay next day. On the day of assay, the media is removed and the cells are incubated with 100 μl of loading buffer (4 μM Fluo4-AM in complete culture media containing 2.5 mM Probenicid, 0.5 mg/ml and 0.2% bovine serum albumin) in 5% CO<sub>2</sub> incubator at 37°C for 1 hr. The loading buffer is removed, and the cells are washed with wash buffer (Hank's Balanced Salt Solution containing 2.5 mM Probenicid, 20 mM HEPES, 0.5 mg/ml and 0.2% bovine



serum albumin, pH 7.4)). One hundred fifty  $\mu$ l of wash buffer containing various concentrations of test compound are added to the cells, and the cells are incubated in 5% CO<sub>2</sub> incubator at 37°C for 30 min. Fifty  $\mu$ l of wash buffer containing various concentration of MCH are added to each well, and transient changes in [Ca<sup>2+</sup>]<sub>i</sub> evoked by MCH are monitored using the FLIPR or FDSS in 96 well plates at Ex. 488 nm and Em. 530 nm for 290 second. When antagonist activity of compound is tested, 50 nM of MCH is used.

Use of FLIPR™ and FDSS6000™ can be accomplished by following manufacturer's instruction (Molecular Device Corporation and HAMAMATSU Photonics K.K.).

The results were shpwn below.

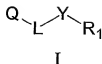
| Compound No. | IC <sub>50</sub> value (nM) |
|--------------|-----------------------------|
| Example 41   | 6                           |
| Example 42   | 19                          |

It is intended that each of the patents, applications, printed publications, and other published documents mentioned or referred to in this specification be herein incorporated by reference in their entirety.

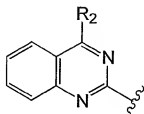
Those skilled in the art will appreciate that numerous changes and modifications may be made to the preferred embodiments of the invention and that such changes and modifications may be made without departing from the spirit of the invention. It is therefore intended that the appended claims cover all such equivalent variations as fall within the true spirit and scope of the invention.

**What is claimed is:**

1. A compound of Formula I:



wherein Q is



II

or



III

R<sub>1</sub> represents

(i) C<sub>1</sub>-C<sub>16</sub> alkyl,

C<sub>1</sub>-C<sub>16</sub> alkyl substituted by substituent(s) independently selected from

- halogen,
- hydroxy,
- oxo,
- C<sub>1</sub>-C<sub>3</sub> alkoxy,
- C<sub>1</sub>-C<sub>3</sub> alkoxy substituted by substituent(s) independently selected from
  - carbocyclic aryl,
  - heterocyclyl,
  - heterocyclyl substituted by C<sub>1</sub>-C<sub>3</sub> alkyl,
- C<sub>1</sub>-C<sub>3</sub> alkylcarbonyloxy,
- carbocyclyloxy,
- carbocyclic aryloxy,
- carbocyclic aryloxy substituted by substituent(s) independently selected from
  - halogen,
  - nitro,
  - carbocyclic aryl,
- carbocyclic aryl substituted by C<sub>1</sub>-C<sub>3</sub> alkoxy,

- C<sub>1</sub>-C<sub>4</sub> alkyl,
- C<sub>1</sub>-C<sub>4</sub> alkyl substituted by substituent(s) independently selected from
  - oxo,
  - mono- or di-C<sub>1</sub>-C<sub>3</sub> alkylamino,
  - mono- or di-C<sub>1</sub>-C<sub>3</sub> alkylamino substituted by carbocyclic aryl,
  - mono- or di-C<sub>1</sub>-C<sub>3</sub> alkylamino substituted by halogenated carbocyclic aryl,
  - carbocyclic arylcarbonylamino,
  - halogenated carbocyclic arylcarbonylamino,
  - heterocyclyloxy,
  - heterocyclyloxy substituted by C<sub>1</sub>-C<sub>3</sub> alkyl,
  - substituted heterocyclyl-ethylideneaminooxy,
  - C<sub>1</sub>-C<sub>3</sub> alkoxycarbonyl,
  - C<sub>1</sub>-C<sub>3</sub> alkoxycarbonyl substituted by carbocyclic aryl,
  - mono- or di-C<sub>1</sub>-C<sub>3</sub> alkylaminocarbonyl,
  - mono- or di-C<sub>1</sub>-C<sub>3</sub> alkylamino,
  - mono- or di-C<sub>1</sub>-C<sub>3</sub> alkylamino substituted by substituent(s) independently selected from
    - cyano,
    - carbocyclic aryl,
    - heterocyclyl,
    - mono- or di-carbocyclic arylamino,
    - mono- or di-carbocyclic arylamino substituted by substituent(s) independently selected from
      - hydroxy,
      - C<sub>1</sub>-C<sub>3</sub> alkyl,
      - C<sub>1</sub>-C<sub>3</sub> alkylcarbonylamino,
      - C<sub>1</sub>-C<sub>3</sub> alkylcarbonylamino substituted by substituent(s) independently selected from
        - C<sub>1</sub>-C<sub>3</sub> alkylcarbonylamino,
        - carbocyclic arylcarbonylamino,
        - heterocyclyl,
        - C<sub>1</sub>-C<sub>4</sub> alkoxycarbonylamino,
        - heterocyclyl carbonylamino,
        - carbocyclic arylsulfonylamino,

- carbocyclic arylsulfonylamino substituted by substituent(s) independently selected from
  - nitro,
  - C<sub>1</sub>-C<sub>3</sub> alkyl,
  - mono- or di-C<sub>1</sub>-C<sub>3</sub> alkylamino,
  - C<sub>1</sub>-C<sub>3</sub> alkylthio,
  - C<sub>1</sub>-C<sub>3</sub> alkylthio substituted by substituent(s) independently selected from
    - mono- or di-carbocyclic arylaminocarbonyl,
    - halogenated mono- or di-carbocyclic arylaminocarbonyl,
    - mono- or di-carbocyclic arylamino,
    - halogenated mono- or di-carbocyclic arylamino,
    - carbocyclic aryl,
    - carbocyclic aryl substituted by substituent(s) independently selected from
      - halogen,
      - C<sub>1</sub>-C<sub>3</sub> alkoxy,
  - carbocyclic arylthio,
  - carbocyclic arylthio substituted by substituent(s) independently selected from
    - halogen,
    - C<sub>1</sub>-C<sub>3</sub> alkyl,
  - carbocyclic arylsulfonyl,
  - halogenated carbocyclic arylsulfonyl,
  - heterocyclylthio,
  - heterocyclylthio substituted by substituent(s) independently selected from
    - nitro,
    - C<sub>1</sub>-C<sub>3</sub> alkyl,
  - C<sub>3</sub>-C<sub>6</sub> cycloalkyl,
  - C<sub>3</sub>-C<sub>6</sub> cycloalkyl substituted by C<sub>1</sub>-C<sub>3</sub> alkyl,
  - C<sub>3</sub>-C<sub>6</sub> cycloalkenyl,
  - carbocyclyl,
  - carbocyclyl substituted by substituent(s) independently selected from
    - halogen,
    - C<sub>1</sub>-C<sub>3</sub> alkyl,
    - C<sub>1</sub>-C<sub>3</sub> alkoxy,

- C<sub>2</sub>-C<sub>3</sub> alkenyl,
- C<sub>2</sub>-C<sub>3</sub> alkenyl substituted by carbocyclic aryl,
- C<sub>2</sub>-C<sub>3</sub> alkenyl substituted by carbocyclic aryl substituted C<sub>1</sub>-C<sub>3</sub> alkylsulfinyl,
- carbocyclic aryl,
- carbocyclic aryl substituted by substituent(s) independently selected from
  - halogen,
  - hydroxy,
  - nitro,
  - C<sub>1</sub>-C<sub>4</sub> alkyl,
  - C<sub>1</sub>-C<sub>4</sub> alkyl substituted by substituent(s) independently selected from
    - halogen,
    - hydroxy,
    - oxo,
    - carbocyclic aryl,
    - heterocyclyl,
    - mono- or di-carbocyclic arylamino,
    - mono- or di-carbocyclic arylamino substituted by substituent(s) independently selected from
      - halogen,
      - nitro,
      - C<sub>1</sub>-C<sub>3</sub> alkyl,
      - C<sub>1</sub>-C<sub>3</sub> alkoxy,
      - halogenated C<sub>1</sub>-C<sub>3</sub> alkoxy,
      - C<sub>1</sub>-C<sub>4</sub> alkoxy,
      - C<sub>1</sub>-C<sub>4</sub> alkoxy substituted by substituent(s) independently selected from
        - halogen,
        - carbocyclic aryl,
        - carbocyclic aryloxy,
        - C<sub>1</sub>-C<sub>3</sub> alkoxycarbonyl,
        - C<sub>1</sub>-C<sub>3</sub> alkylcarbonyloxy,
        - mono- or di-C<sub>1</sub>-C<sub>3</sub> alkylamino,
        - mono- or di-carbocyclic arylamino,

- halogenated mono- or di-carbocyclic arylamino,
- mono- or di-carbocyclic arylaminocarbonyl,
- mono- or di-carbocyclic arylaminocarbonyl substituted by substituent(s) independently selected from
  - halogen,
  - nitro,
  - C<sub>1</sub>-C<sub>3</sub> alkyl,
  - C<sub>1</sub>-C<sub>3</sub> alkoxy,
  - halogenated C<sub>1</sub>-C<sub>3</sub> alkoxy,
  - mercapto,
  - C<sub>1</sub>-C<sub>3</sub> alkylthio,
  - halogenated C<sub>1</sub>-C<sub>3</sub> alkylthio,
  - C<sub>1</sub>-C<sub>3</sub> alkylsulfonyl,
  - C<sub>3</sub>-C<sub>6</sub> cycloalkyl,
  - carbocyclic aryl,
  - heterocyclyl,
  - heterocyclyl,
  - heterocyclyl substituted by substituent(s) independently selected from
    - hydroxy,
    - C<sub>1</sub>-C<sub>3</sub> alkyl,
    - C<sub>1</sub>-C<sub>3</sub> alkyl substituted by carbocyclic aryl,
    - C<sub>1</sub>-C<sub>3</sub> alkoxy,
    - C<sub>1</sub>-C<sub>3</sub> alkoxy substituted by carbocyclic aryl,
    - carbocyclic aryl,
    - halogenated carbocyclic aryl,
- (ii) C<sub>2</sub>-C<sub>8</sub> alkenyl,  
C<sub>2</sub>-C<sub>8</sub> alkenyl substituted by substituent(s) independently selected from
  - halogen,
  - oxo,
  - C<sub>1</sub>-C<sub>3</sub> alkoxy,
  - C<sub>1</sub>-C<sub>3</sub> alkoxy substituted by carbocyclic aryl,
  - carbocyclic aryl,

- carbocyclic aryl substituted by substituent(s) independently selected from
  - halogen,
  - hydroxy,
  - nitro,
  - C<sub>1</sub>-C<sub>3</sub> alkyl,
  - halogenated C<sub>1</sub>-C<sub>3</sub> alkyl,
  - C<sub>1</sub>-C<sub>3</sub> alkoxy,
  - halogenated C<sub>1</sub>-C<sub>3</sub> alkoxy,
  - heterocyclyl,
  - heterocyclyl substituted by substituent(s) independently selected from
    - hydroxy,
    - nitro,
    - C<sub>1</sub>-C<sub>3</sub> alkyl,
    - C<sub>1</sub>-C<sub>3</sub> alkoxy,
- (iii) C<sub>2</sub>-C<sub>4</sub> alkynyl,  
C<sub>2</sub>-C<sub>4</sub> alkynyl substituted by carbocyclic aryl,
- (iv) C<sub>3</sub>-C<sub>6</sub> cycloalkyl,  
C<sub>3</sub>-C<sub>6</sub> cycloalkyl substituted by substituent(s) independently selected from
  - C<sub>1</sub>-C<sub>3</sub> alkyl,
  - C<sub>1</sub>-C<sub>3</sub> alkyl substituted by substituent(s) independently selected from
    - hydroxy,
    - oxo,
    - carbocyclic aryl,
    - mono- or di-C<sub>1</sub>-C<sub>3</sub> alkylamino,
    - mono- or di-C<sub>1</sub>-C<sub>3</sub> alkylamino substituted by carbocyclic aryl,
    - carbocyclic arylcarbonylamino,
    - carbocyclic aryl,
- (v) C<sub>3</sub>-C<sub>6</sub> cycloalkenyl,  
C<sub>3</sub>-C<sub>6</sub> cycloalkenyl substituted by C<sub>1</sub>-C<sub>3</sub> alkyl,
- (vi) carbocyclyl,  
carbocyclyl substituted by substituent(s) independently selected from
  - hydroxy,

- nitro,
- (vii) carbocyclic aryl,
- carbocyclic aryl substituted by substituent(s) independently selected from
  - halogen,
  - hydroxy,
  - cyano,
  - nitro,
  - C<sub>1</sub>-C<sub>9</sub> alkyl,
  - C<sub>1</sub>-C<sub>9</sub> alkyl substituted by substituent(s) independently selected from
    - halogen,
    - hydroxy,
    - oxo,
    - C<sub>1</sub>-C<sub>3</sub> alkoxy,
    - carbocyclic aryloxy,
    - mono- or di-C<sub>1</sub>-C<sub>3</sub> alkylamino-N-oxy,
    - mono- or di-C<sub>1</sub>-C<sub>3</sub> alkylamino,
    - mono- or di-C<sub>1</sub>-C<sub>3</sub> alkylamino substituted by carbocyclic aryl,
    - mono- or di-carbocyclic arylamino,
    - carbocyclylimino,
    - carbocyclylimino substituted by carbocyclic aryl,
    - mono- or di-carbocyclic arylamino,
    - mono- or di-carbocyclic arylamino substituted by C<sub>1</sub>-C<sub>3</sub> alkoxy,
    - mono- or di-carbocyclic arylaminocarbonyl,
    - mono- or di-carbocyclic arylaminocarbonyl substituted by C<sub>1</sub>-C<sub>3</sub> alkoxy,
    - carbocyclic aryl,
    - carbocyclic aryl substituted by substituent(s) independently selected from
      - halogen,
      - C<sub>1</sub>-C<sub>3</sub> alkyl,
      - halogenated C<sub>1</sub>-C<sub>3</sub> alkyl,
      - heterocyclyl,
      - heterocyclyl substituted by C<sub>1</sub>-C<sub>3</sub> alkyl,
      - C<sub>2</sub>-C<sub>3</sub> alkenyl,



- C<sub>2</sub>-C<sub>3</sub> alkenyl substituted by carbocyclic aryl,
- C<sub>1</sub>-C<sub>9</sub> alkoxy,
- C<sub>1</sub>-C<sub>9</sub> alkoxy substituted by substituent(s) independently selected from
  - hydroxy,
  - halogen,
  - carboxy,
  - mono- or di-C<sub>1</sub>-C<sub>3</sub> alkylamino,
  - carbocyclic aryl,
  - halogenated carbocyclic aryl,
  - heterocyclyl,
  - heterocyclyl substituted by substituent(s) independently selected from
    - halogen,
    - heterocyclyl,
    - heterocyclyl substituted by substituent(s) independently selected from
      - halogen,
      - C<sub>1</sub>-C<sub>3</sub> alkyl,
      - halogenated C<sub>1</sub>-C<sub>3</sub> alkyl,
- C<sub>2</sub>-C<sub>3</sub> alkenyloxy,
- C<sub>1</sub>-C<sub>3</sub> alkylcarbonyloxy,
- carbocyclic aryloxy,
- carbocyclic aryloxy substituted by substituent(s) independently selected from
  - halogen,
  - nitro,
  - C<sub>1</sub>-C<sub>4</sub> alkyl,
  - halogenated C<sub>1</sub>-C<sub>4</sub> alkyl,
  - C<sub>1</sub>-C<sub>3</sub> alkoxy,
  - heterocyclyloxy,
  - heterocyclyloxy substituted by substituent(s) independently selected from
    - halogen,
    - C<sub>1</sub>-C<sub>3</sub> alkyl,
    - halogenated C<sub>1</sub>-C<sub>3</sub> alkyl,
- (carbocyclic aryl)S(O)<sub>2</sub>O,

- carboxy,
- C<sub>1</sub>-C<sub>3</sub> alkoxy carbonyl,
- mono- or di-C<sub>1</sub>-C<sub>3</sub> alkylaminocarbonyl,
- mono- or di-C<sub>1</sub>-C<sub>3</sub> alkylaminocarbonyl substituted by carbocyclic aryl,
- mono- or di-carbocyclic arylaminocarbonyl,
- mono- or di-carbocyclic arylaminocarbonyl substituted by C<sub>1</sub>-C<sub>3</sub> alkyl,
- amino,
- mono- or di-C<sub>1</sub>-C<sub>4</sub> alkylamino,
- mono- or di-C<sub>1</sub>-C<sub>4</sub> alkylamino substituted by cyano,
- mono- or di-carbocyclic arylamino,
- C<sub>1</sub>-C<sub>3</sub> alkynylcarbonylamino,
- C<sub>1</sub>-C<sub>3</sub> alkynylcarbonylamino substituted by carbocyclic aryl,
- carbocyclic arylsulfonylamino,
- carbocyclic arylsulfonylamino substituted by C<sub>1</sub>-C<sub>3</sub> alkyl,
- (carbocyclic aryl)NHC(O)NH,
- (carbocyclic aryl)NHC(O)NH substituted by C<sub>1</sub>-C<sub>3</sub> alkoxy,
- (carbocyclic aryl)NHC(O)NH substituted by halogenated C<sub>1</sub>-C<sub>3</sub> alkoxy,
- carbocyclic aryl diazo,
- carbocyclic aryl diazo substituted by mono- or di- C<sub>1</sub>-C<sub>3</sub> alkylamino,
- C<sub>1</sub>-C<sub>3</sub> alkylthio,
- halogenated C<sub>1</sub>-C<sub>3</sub> alkylthio,
- carbocyclic arylthio,
- carbocyclic arylthio substituted by substituent(s) independently selected from
  - halogen,
  - cyano,
  - C<sub>1</sub>-C<sub>3</sub> alkyl,
  - heterocyclylthio,
  - C<sub>1</sub>-C<sub>3</sub> alkylsulfonyl,
  - mono- or di-C<sub>1</sub>-C<sub>3</sub> alkylaminosulfonyl,
  - carbocyclic aryl,
  - carbocyclic aryl substituted by substituent(s) independently selected from
    - C<sub>1</sub>-C<sub>7</sub> alkyl,

- halogenated C<sub>1</sub>-C<sub>7</sub> alkyl,
- heterocyclyl,
- heterocyclyl substituted by substituent(s) independently selected from
  - C<sub>1</sub>-C<sub>3</sub> alkyl,
  - carbocyclic aryl,
  - halogenated carbocyclic aryl,
- (viii) heterocyclyl,  
or heterocyclyl substituted by substituent(s) independently selected from
  - halogen,
  - hydroxy,
  - cyano,
  - nitro,
  - C<sub>1</sub>-C<sub>4</sub> alkyl,
  - C<sub>1</sub>-C<sub>4</sub> alkyl substituted by substituent(s) independently selected from
    - halogen,
    - hydroxy,
    - oxo,
    - C<sub>1</sub>-C<sub>3</sub> alkylcarbonyloxy,
    - carbocyclic arylcarbonylamino,
    - halogenated carbocyclic arylcarbonylamino,
    - C<sub>1</sub>-C<sub>3</sub> alkoxycarbonyl,
    - C<sub>1</sub>-C<sub>3</sub> alkylthio,
    - C<sub>1</sub>-C<sub>3</sub> alkylthio substituted by carbocyclic aryl,
    - C<sub>1</sub>-C<sub>3</sub> alkylthio substituted by halogenated carbocyclic aryl,
  - carbocyclic aryl,
  - carbocyclic aryl substituted by substituent(s) independently selected from
    - halogen,
    - nitro,
    - heterocyclyl,
    - heterocyclyl substituted by substituent(s) independently selected from
      - halogen,
      - C<sub>1</sub>-C<sub>3</sub> alkyl,

- halogenated C<sub>1</sub>-C<sub>3</sub> alkyl,
- C<sub>1</sub>-C<sub>3</sub> alkoxy,
- C<sub>1</sub>-C<sub>3</sub> alkoxy substituted by carbocyclic aryl,
- carbocyclic aryloxy,
- carbocyclic aryloxy substituted by substituent(s) independently selected from
  - halogen,
  - C<sub>1</sub>-C<sub>3</sub> alkyl,
  - mono- or di-C<sub>1</sub>-C<sub>3</sub> alkylamino,
  - C<sub>1</sub>-C<sub>4</sub> alkylcarbonylamino,
  - C<sub>1</sub>-C<sub>3</sub> alkylthio,
  - C<sub>1</sub>-C<sub>3</sub> alkenylthio,
  - carbocyclic arylthio,
  - halogenated carbocyclic arylthio,
  - carbocyclic arylthio substituted by C<sub>1</sub>-C<sub>3</sub> alkoxy carbonyl,
  - heterocyclylthio,
  - heterocyclylthio substituted by C<sub>1</sub>-C<sub>3</sub> alkyl,
  - C<sub>1</sub>-C<sub>3</sub> alkylsulfonyl,
  - carbocyclic arylsulfonyl,
  - halogenated carbocyclic arylsulfonyl,
  - carbocyclic arylsulfonyl substituted by C<sub>1</sub>-C<sub>4</sub> alkyl,
  - C<sub>1</sub>-C<sub>3</sub> alkoxy carbonyl,
  - carbocyclic aryl,
  - carbocyclic aryl substituted by substituent(s) independently selected from
    - halogen,
    - nitro,
    - C<sub>1</sub>-C<sub>3</sub> alkyl,
    - halogenated C<sub>1</sub>-C<sub>3</sub> alkyl,
    - C<sub>1</sub>-C<sub>3</sub> alkoxy,
    - halogenated C<sub>1</sub>-C<sub>3</sub> alkoxy,
    - heterocyclyl,
    - heterocyclyl substituted by substituent(s) independently selected from
      - halogen,

- C<sub>1</sub>-C<sub>3</sub> alkyl,
- halogenated C<sub>1</sub>-C<sub>3</sub> alkyl,
- C<sub>1</sub>-C<sub>3</sub> alkoxy,
- C<sub>1</sub>-C<sub>3</sub> alkoxycarbonyl;

R<sub>2</sub> is -NHNH<sub>2</sub>, -NHNHBoc, -N(R<sub>2a</sub>)(R<sub>2b</sub>), morpholino, 4-acetyl-piperazyl, or 4-phenyl-piperazyl;

wherein R<sub>2a</sub> is H or C<sub>1</sub>-C<sub>3</sub> alkyl;

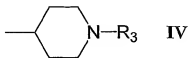
R<sub>2b</sub> is C<sub>1</sub>-C<sub>4</sub> alkyl, C<sub>1</sub>-C<sub>4</sub> alkyl substituted by substituent(s) independently selected from

- hydroxy,
- C<sub>1</sub>-C<sub>3</sub> alkoxy,
- amino,
- NHBoc,
- C<sub>3</sub>-C<sub>6</sub> cycloalkyl,
- carbocyclic aryl,
- carbocyclic aryl substituted by substituent(s) independently selected from
- halogen,
- C<sub>1</sub>-C<sub>3</sub> alkyl,
- C<sub>1</sub>-C<sub>3</sub> alkoxy,
- SO<sub>2</sub>NH<sub>2</sub>,
- heterocyclyl,

C<sub>3</sub>-C<sub>6</sub> cycloalkyl, carbocyclic aryl, carbocyclic aryl substituted by substituent(s) independently selected from

- halogen,
- C<sub>1</sub>-C<sub>3</sub> alkyl,
- C<sub>1</sub>-C<sub>3</sub> alkoxy,

or a group of Formula IV;

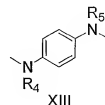
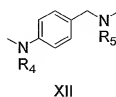
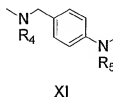
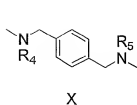
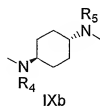
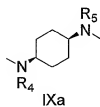
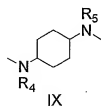
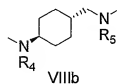
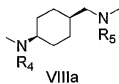
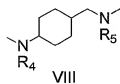
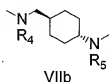
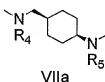
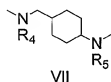
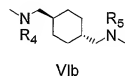
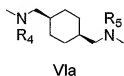
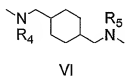
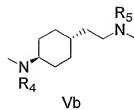
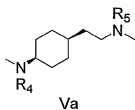
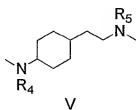


wherein Boc is carbamic acid *tert*-butyl ester and R<sub>3</sub> is C<sub>1</sub>-C<sub>3</sub> alkyl or C<sub>1</sub>-C<sub>3</sub> alkyl

substituted by substituent(s) independently selected from

- carbocyclic aryl,
- halogenated carbocyclic aryl,
- carbocyclic aryl substituted by C<sub>1</sub>-C<sub>3</sub> alkoxy;

L is selected from Formula V - XIX;





XIV



XV



XVI



XVII



XVIII



XIX

wherein  $R_4$  is H or  $C_1$ - $C_3$  alkyl;

$R_5$  is H,  $C_1$ - $C_3$  alkyl, or  $C_1$ - $C_3$  alkyl substituted by a substituted carbocyclic aryl;

Y is  $-S(O)_2-$ ,  $-C(O)-$ , or  $-(CH_2)_m$ ;

m is 0 or 1;

wherein carbocyclic aryl is phenyl, naphthyl, anthranyl, biphenyl, or phenanthryl;

carbocyclyl is 10,11-dihydro-5-oxo-dibenzo[a,d]cycloheptyl, 1-oxo-indanyl, 7,7-dimethyl-2-oxo-bicyclo[2.2.1]heptyl, 9H-fluorenyl, 9-oxo-fluorenyl, acenaphthyl, anthraquinonyl, C-fluorene-9-ylidene, indanyl, indenyl, 1,2,3,4-tetrahydro-naphthyl, or bicyclo[2.2.1]hepteny;

heterocycl is 1,2,3,4-tetrahydro-isoquinolyl, 1,2,3-thiadiazolyl, 1,2,3-triazolyl, 1,2-dihydro-3-oxo-pyrazolyl, 1,3,4-thiadiazolyl, 1,3-dioxo-isindolyl, 1,3-dioxolanyl, 1H-indolyl, 1H-pyrrolo[2,3-c]pyridyl, 1H-pyrrolyl, 1-oxo-3H-isobenzofuranyl, 2,2',5',2"-terthiophenyl, 2,2'-bithiophenyl, 2,3-dihydro-1-oxo-isindolyl, 2,3-dihydro-benzo[1,4]dioxinyl, 2,4-dihydro-3-oxo-pyrazolyl, 2H-benzopyranyl, 2-oxo-benzopyranyl, 2-oxo-pyrrolidinyl, 3,4-dihydro-2H-benzo[1,4]oxazinyl, 3,4-dihydro-2H-benzo[b][1,4]dioxepinyl, 4H-benzo[1,3]dioxinyl, 4H-benzopyranyl, 4-oxo-1,5,6,7-tetrahydro-indolyl, 4-oxo-3,4-dihydro-phthalazinyl, 4-oxo-benzopyranyl, 9,10,10-trioxo-thioxanthenyl, 9H-carbazolyl, 9H-xanthenyl, azetidiny, benzimidazolyl, benzo[1,3]dioxolyl, benzo[2,1,3]oxadiazolyl, benzo[b]thienyl, benzofuryl, benzothiazolyl, cinnolyl, furyl, imidazo[2,1-b]thiazolyl, imidazolyl, isoxazolyl, morpholino, morpholinyl, oxazolyl, oxolanyl, piperazyl, piperidyl, piridyl, pyrazolo[5,1-b]thiazolyl, pyrazolyl, pyridyl, pyrimidyl, pyrrolidyl, quinolyl, quinoxalyl, thiazolidyl, thiazolyl, thienyl, thiolanyl, 2,3-

dihydro-benzofuryl, tetrahydro-thienyl, or benzofuranyl;

halogen is fluoro, chloro, bromo, or iodo;

or a salt thereof.

2. A compound according to claim 1, wherein Q is Fomura II;

R<sub>1</sub> represents

(i) C<sub>1</sub>-C<sub>10</sub> alkyl,

C<sub>1</sub>-C<sub>10</sub> alkyl substituted by substituent(s) independently selected from

•halogen,

•oxo,

•C<sub>1</sub>-C<sub>3</sub> alkoxy,

•C<sub>1</sub>-C<sub>3</sub> alkoxy substituted by carbocyclic aryl,

•C<sub>1</sub>-C<sub>3</sub> alkylcarbonyloxy,

•carbocyclyloxy,

•carbocyclic aryloxy,

•carbocyclic aryloxy substituted by substituent(s) independently selected from

••halogen,

••nitro,

••C<sub>1</sub>-C<sub>4</sub> alkyl,

••C<sub>1</sub>-C<sub>4</sub> alkyl substituted by substituent(s) independently selected from

•••oxo,

•••carbocyclic arylcarbonylamino,

•••halogenated carbocyclic arylcarbonylamino,

•heterocyclyloxy,

•heterocyclyloxy substituted by C<sub>1</sub>-C<sub>3</sub> alkyl,

•substituted heterocyclyl-ethylideneaminoxy,

•C<sub>1</sub>-C<sub>3</sub> alkoxycarbonyl,

•C<sub>1</sub>-C<sub>3</sub> alkoxycarbonyl substituted by carbocyclic aryl,

•mono- or di-C<sub>1</sub>-C<sub>3</sub> alkylaminocarbonyl,

•mono- or di-carbocyclic arylamino,

•mono- or di-carbocyclic arylamino substituted by hydroxy,

•C<sub>1</sub>-C<sub>3</sub> alkylcarbonylamino,



- C<sub>1</sub>-C<sub>3</sub> alkylcalbonylamino substituted by substituent(s) independently selected from
  - C<sub>1</sub>-C<sub>3</sub> alkylcalbonylamino,
  - carbocyclic arylcalbonylamino,
  - heterocyclyl,
- C<sub>1</sub>-C<sub>4</sub> alkoxycalbonylamino,
- heterocyclyl calbonylamino,
- carbocyclic arylsulfonylamino,
- carbocyclic arylsulfonylamino substituted by substituent(s) independently selected from
  - nitro,
  - C<sub>1</sub>-C<sub>3</sub> alkyl,
  - mono- or di-C<sub>1</sub>-C<sub>3</sub> alkylamino,
  - C<sub>1</sub>-C<sub>3</sub> alkylthio,
  - C<sub>1</sub>-C<sub>3</sub> alkylthio substituted by substituent(s) independently selected from
    - mono- or di-carbocyclic arylaminocarbonyl,
    - halogenated mono- or di-carbocyclic arylaminocarbonyl,
    - carbocyclic aryl,
    - carbocyclic aryl substituted by substituent(s) independently selected from
      - halogen,
      - C<sub>1</sub>-C<sub>3</sub> alkoxy,
    - carbocyclic arylthio,
    - carbocyclic arylthio substituted by substituent(s) independently selected from
      - halogen,
      - C<sub>1</sub>-C<sub>3</sub> alkyl,
    - carbocyclic arylsulfonyl,
    - halogenated carbocyclic arylsulfonyl,
    - heterocyclylthio,
    - heterocyclylthio substituted by substituent(s) independently selected from
      - nitro,
      - C<sub>1</sub>-C<sub>3</sub> alkyl,
    - C<sub>3</sub>-C<sub>6</sub> cycloalkyl,
    - C<sub>3</sub>-C<sub>6</sub> cycloalkyl substituted by C<sub>1</sub>-C<sub>3</sub> alkyl,
    - C<sub>3</sub>-C<sub>6</sub> cycloalkenyl,

- carbocyclyl,
- carbocyclyl substituted by substituent(s) independently selected from
  - halogen,
  - C<sub>1</sub>-C<sub>3</sub> alkyl,
  - C<sub>1</sub>-C<sub>3</sub> alkoxy,
  - C<sub>2</sub>-C<sub>3</sub> alkenyl,
  - C<sub>2</sub>-C<sub>3</sub> alkenyl substituted by carbocyclic aryl,
  - C<sub>2</sub>-C<sub>3</sub> alkenyl substituted by carbocyclic aryl substituted C<sub>1</sub>-C<sub>3</sub> alkylsulfinyl,
  - carbocyclic aryl,
  - carbocyclic aryl substituted by substituent(s) independently selected from
    - halogen,
    - hydroxy,
    - nitro,
    - C<sub>1</sub>-C<sub>4</sub> alkyl,
    - C<sub>1</sub>-C<sub>4</sub> alkyl substituted by substituent(s) independently selected from
      - oxo,
      - carbocyclic aryl,
      - heterocyclyl,
      - C<sub>1</sub>-C<sub>4</sub> alkoxy,
      - C<sub>1</sub>-C<sub>4</sub> alkoxy substituted by substituent(s) independently selected from
        - halogen,
        - carbocyclic aryl,
        - carbocyclic aryloxy,
        - C<sub>1</sub>-C<sub>3</sub> alkylcarbonyloxy,
        - mono- or di-carbocyclic arylamino,
        - halogenated mono- or di-carbocyclic arylamino,
        - mono- or di-carbocyclic arylaminocarbonyl,
        - mono- or di-carbocyclic arylaminocarbonyl substituted by substituent(s) independently selected from
          - halogen,
          - nitro,
          - C<sub>1</sub>-C<sub>3</sub> alkyl,

- C<sub>1</sub>-C<sub>3</sub> alkoxy,
- halogenated C<sub>1</sub>-C<sub>3</sub> alkoxy,
- mercapto,
- C<sub>1</sub>-C<sub>3</sub> alkylthio,
- halogenated C<sub>1</sub>-C<sub>3</sub> alkylthio,
- C<sub>1</sub>-C<sub>3</sub> alkylsulfonyl,
- C<sub>3</sub>-C<sub>6</sub> cycloalkyl,
- carbocyclic aryl,
- heterocyclyl,
- heterocyclyl,
- heterocyclyl substituted by substituent(s) independently selected from
- hydroxy,
- C<sub>1</sub>-C<sub>3</sub> alkyl,
- C<sub>1</sub>-C<sub>3</sub> alkyl substituted by carbocyclic aryl,
- C<sub>1</sub>-C<sub>3</sub> alkoxy,
- C<sub>1</sub>-C<sub>3</sub> alkoxy substituted by carbocyclic aryl,
- carbocyclic aryl,
- halogenated carbocyclic aryl,

(ii) C<sub>2</sub>-C<sub>6</sub> alkenyl,

C<sub>2</sub>-C<sub>6</sub> alkenyl substituted by substituent(s) independently selected from

- oxo,
- carbocyclic aryl,
- carbocyclic aryl substituted by substituent(s) independently selected from
- halogen,
- nitro,
- C<sub>1</sub>-C<sub>3</sub> alkyl,
- halogenated C<sub>1</sub>-C<sub>3</sub> alkyl,
- C<sub>1</sub>-C<sub>3</sub> alkoxy,
- halogenated C<sub>1</sub>-C<sub>3</sub> alkoxy,
- heterocyclyl,
- heterocyclyl substituted by substituent(s) independently selected from
- hydroxy,

- C<sub>1</sub>-C<sub>3</sub> alkyl,
- C<sub>1</sub>-C<sub>3</sub> alkoxy,
- (iii) C<sub>3</sub>-C<sub>6</sub> cycloalkyl,  
C<sub>3</sub>-C<sub>6</sub> cycloalkyl substituted by substituent(s) independently selected from
  - C<sub>1</sub>-C<sub>3</sub> alkyl,
  - C<sub>1</sub>-C<sub>3</sub> alkyl substituted by substituent(s) independently selected from
    - oxo,
    - carbocyclic aryl,
    - carbocyclic arylcarbonylamino,
    - carbocyclic aryl,
    - (iv) carbocyclyl,  
carbocyclyl substituted by nitro,
    - (v) carbocyclic aryl,  
carbocyclic aryl substituted by substituent(s) independently selected from
      - halogen,
      - hydroxy,
      - cyano,
      - nitro,
      - C<sub>1</sub>-C<sub>9</sub> alkyl,
      - C<sub>1</sub>-C<sub>9</sub> alkyl substituted by substituent(s) independently selected from
        - halogen,
        - oxo,
        - carbocyclic aryloxy,
        - carbocyclylimino,
        - carbocyclylimino substituted by carbocyclic aryl,
        - mono- or di-carbocyclic arylaminocarbonyl,
        - mono- or di-carbocyclic arylaminocarbonyl substituted by C<sub>1</sub>-C<sub>3</sub> alkoxy,
        - carbocyclic aryl,
        - carbocyclic aryl substituted by substituent(s) independently selected from
          - halogen,
          - C<sub>1</sub>-C<sub>3</sub> alkyl,
          - halogenated C<sub>1</sub>-C<sub>3</sub> alkyl,

- heterocyclyl,
- heterocyclyl substituted by C<sub>1</sub>-C<sub>3</sub> alkyl,
- C<sub>1</sub>-C<sub>7</sub> alkoxy,
- C<sub>1</sub>-C<sub>7</sub> alkoxy substituted by substituent(s) independently selected from
  - halogen,
  - carbocyclic aryl,
  - C<sub>1</sub>-C<sub>3</sub> alkylcarbonyloxy,
  - carbocyclic aryloxy,
  - carbocyclic aryloxy substituted by C<sub>1</sub>-C<sub>3</sub> alkoxy,
  - C<sub>1</sub>-C<sub>3</sub> alkoxycarbonyl,
  - mono- or di-C<sub>1</sub>-C<sub>3</sub> alkylaminocarbonyl,
  - mono- or di-C<sub>1</sub>-C<sub>3</sub> alkylaminocarbonyl substituted by carbocyclic aryl,
  - mono- or di-carbocyclic arylaminocarbonyl,
  - mono- or di-carbocyclic arylaminocarbonyl substituted by C<sub>1</sub>-C<sub>3</sub> alkyl,
  - amino,
  - mono- or di-C<sub>1</sub>-C<sub>3</sub> alkylamino,
  - C<sub>1</sub>-C<sub>3</sub> alkynylcarbonylamino,
  - C<sub>1</sub>-C<sub>3</sub> alkynylcarbonylamino substituted by carbocyclic aryl,
  - carbocyclic arylsulfonylamino,
  - carbocyclic arylsulfonylamino substituted by C<sub>1</sub>-C<sub>3</sub> alkyl,
  - (carbocyclic aryl)NHC(O)NH,
  - (carbocyclic aryl)NHC(O)NH substituted by C<sub>1</sub>-C<sub>3</sub> alkoxy,
  - (carbocyclic aryl)NHC(O)NH substituted by halogenated C<sub>1</sub>-C<sub>3</sub> alkoxy,
  - C<sub>1</sub>-C<sub>3</sub> alkylthio,
  - halogenated C<sub>1</sub>-C<sub>3</sub> alkylthio,
  - carbocyclic arylthio,
  - carbocyclic arylthio substituted by cyano,
  - C<sub>1</sub>-C<sub>3</sub> alkylsulfonyl,
  - mono- or di-C<sub>1</sub>-C<sub>3</sub> alkylaminosulfonyl,
  - carbocyclic aryl,
  - carbocyclic aryl substituted by substituent(s) independently selected from
    - C<sub>1</sub>-C<sub>7</sub> alkyl,

- halogenated C<sub>1</sub>-C<sub>7</sub> alkyl,
- heterocyclyl,
- heterocyclyl substituted by substituent(s) independently selected from
  - C<sub>1</sub>-C<sub>3</sub> alkyl,
  - carbocyclic aryl,
  - halogenated carbocyclic aryl,
- (vi) heterocyclyl,
  - or heterocyclyl substituted by substituent(s) independently selected from
    - halogen,
    - nitro,
    - C<sub>1</sub>-C<sub>4</sub> alkyl,
    - C<sub>1</sub>-C<sub>4</sub> alkyl substituted by substituent(s) independently selected from
      - halogen,
      - oxo,
      - C<sub>1</sub>-C<sub>3</sub> alkylthio,
      - C<sub>1</sub>-C<sub>3</sub> alkylthio substituted by carbocyclic aryl,
      - C<sub>1</sub>-C<sub>3</sub> alkylthio substituted by halogenated carbocyclic aryl,
      - carbocyclic aryl,
      - halogenated carbocyclic aryl,
      - heterocyclyl,
      - C<sub>1</sub>-C<sub>3</sub> alkoxy,
      - carbocyclic aryloxy,
      - carbocyclic aryloxy substituted by substituent(s) independently selected from
        - halogen,
        - C<sub>1</sub>-C<sub>3</sub> alkyl,
        - C<sub>1</sub>-C<sub>3</sub> alkylthio,
        - C<sub>1</sub>-C<sub>3</sub> alkenylthio,
        - carbocyclic arylthio,
        - C<sub>1</sub>-C<sub>3</sub> alkylsulfonyl,
        - carbocyclic arylsulfonyl,
        - halogenated carbocyclic arylsulfonyl,
        - carbocyclic arylsulfonyl substituted by C<sub>1</sub>-C<sub>4</sub> alkyl,

- carbocyclic aryl,
- carbocyclic aryl substituted by substituent(s) independently selected from
- halogen,
- nitro,
- C<sub>1</sub>-C<sub>3</sub> alkyl,
- C<sub>1</sub>-C<sub>3</sub> alkoxy,
- heterocyclyl,
- heterocyclyl substituted by substituent(s) independently selected from
- C<sub>1</sub>-C<sub>3</sub> alkyl,
- halogenated C<sub>1</sub>-C<sub>3</sub> alkyl;

Y is -C(O)-;

wherein carbocyclic aryl is phenyl, naphthyl, anthranyl, or biphenyl;

carbocyclyl is 10,11-dihydro-5-oxo-dibenzo[a,d]cycloheptyl, 1-oxo-indanyl, 9H-fluorenyl, 9-oxo-fluorenyl, acenaphthyl, anthraquinonyl, C-fluoren-9-ylidene, indanyl, indenyl, 1,2,3,4-tetrahydro-naphthyl, or bicyclo[2.2.1]hepteny;

heterocyclyl is 1,2,3-thiadiazolyl, 1,2,3-triazolyl, 1,2-dihydro-3-oxo-pyrazolyl, 1,3-dioxo-isoindolyl, 1H-indolyl, 1H-pyrrolyl, 1-oxo-3H-isobenzofuranyl, 2,3-dihydro-benzo[1,4]dioxinyl, 2,3-dihydro-benzofuryl, 2,4-dihydro-3-oxo-pyrazolyl, 2H-benzopyranyl, 2-oxo-benzopyranyl, 2-oxo-pyrrolidinyl, 3,4-dihydro-2H-benzo[b][1,4]dioxepinyl, 4-oxo-1,5,6,7-tetrahydro-indolyl, 4-oxo-3,4-dihydro-phthalazinyl, 4-oxo-benzopyranyl, 9,10,10-trioxo-thioxanthenyl, 9H-xanthenyl, azetidiny, benzimidazolyl, benzo[1,3]dioxolyl, benzo[2,1,3]oxadiazolyl, benzo[b]thienyl, cinnolyl, furyl, imidazolyl, isoxazolyl, morpholino, morpholinyl, oxazolyl, oxolanyl, piperidyl, piridyl, pyrazolyl, pyridyl, pyrimidyl, pyrrolidyl, quinolyl, quinoxalyl, thiazolidyl, thiazolyl, thienyl, thiolanyl, tetrahydro-thienyl, benzofuranyl, or benzothiazolyl;

halogen is fluoro, chloro, bromo, or iodo;

or a salt thereof.

3. A compound according to claim 2, wherein

R<sub>1</sub> represents

(i) C<sub>1</sub>-C<sub>10</sub> alkyl,

C<sub>1</sub>-C<sub>10</sub> alkyl substituted by substituent(s) independently selected from

- OXO,
- di-propylaminocarbonyl,
- methoxy substituted by carbocyclic aryl,
- methylcarbonyloxy,
- carbocyclic aryloxy,
- halogenated carbocyclic aryloxy,
- carbocyclic aryloxy substituted by nitro,
- heterocyclyloxy substituted by methyl,
- substituted heterocyclyl-ethylideneaminoxy,
- tert*-butoxycarbonylamino,
- carbocyclic arylcarbonylamino,
- C<sub>1</sub>-C<sub>2</sub> alkylthio,
- C<sub>1</sub>-C<sub>2</sub> alkylthio substituted by substituent(s) independently selected from
  - halogenated carbocyclic aryl,
  - carbocyclic aryl substituted by methoxy,
  - carbocyclic arylthio,
  - heterocyclylthio substituted by nitro,
  - heterocyclylthio substituted by methyl,
  - C<sub>5</sub>-C<sub>6</sub> cycloalkyl,
  - C<sub>5</sub>-C<sub>6</sub> cycloalkenyl,
  - carbocyclyl substituted by substituent(s) independently selected from
    - halogen,
    - methyl,
    - methoxy,
    - ethenyl substituted by carbocyclic aryl substituted methylsulfinyl,
    - carbocyclic aryl,
    - carbocyclic aryl substituted by substituent(s) independently selected from
      - halogen,
      - hydroxy,
      - nitro,
      - C<sub>1</sub>-C<sub>4</sub> alkyl,
      - C<sub>1</sub>-C<sub>4</sub> alkyl substituted by substituent(s) independently selected from



- oxo,
- carbocyclic aryl,
- heterocyclyl,
- C<sub>1</sub>-C<sub>4</sub> alkoxy,
- halogenated C<sub>1</sub>-C<sub>4</sub> alkoxy,
- C<sub>1</sub>-C<sub>4</sub> alkoxy substituted by carbocyclic aryl,
- carbocyclic aryloxy,
- halogenated mono-carbocyclic arylaminocarbonyl,
- carbocyclic aryl,
- heterocyclyl,
- heterocyclyl,
- heterocyclyl substituted by substituent(s) independently selected from
- C<sub>1</sub>-C<sub>2</sub> alkyl,
- C<sub>1</sub>-C<sub>2</sub> substituted by carbocyclic aryl,
- methoxy,
- methoxy substituted by carbocyclic aryl,
- carbocyclic aryl,
- halogenated carbocyclic aryl,
- (ii) C<sub>2</sub>-C<sub>3</sub> alkenyl substituted by substituent(s) independently selected from
  - carbocyclic aryl,
  - halogenated carbocyclic aryl,
  - carbocyclic aryl substituted by nitro,
- (iii) C<sub>3</sub>-C<sub>6</sub> cycloalkyl,  
C<sub>3</sub>-C<sub>6</sub> cycloalkyl substituted by substituent(s) independently selected from
  - methyl substituted by oxo,
  - methyl substituted by carbocyclic aryl,
  - carbocyclic aryl,
- (iv) carbocyclyl,
- (v) carbocyclic aryl,  
carbocyclic aryl substituted by substituent(s) independently selected from
  - halogen,
  - hydroxy,

- cyano,
- nitro,
- C<sub>1</sub>-C<sub>9</sub> alkyl,
- C<sub>1</sub>-C<sub>9</sub> alkyl substituted by substituent(s) independently selected from
  - halogen,
  - oxo,
  - carbocyclic aryl,
  - carbocyclic aryl substituted by methyl,
  - carbocyclic aryloxy,
  - C<sub>1</sub>-C<sub>7</sub> alkoxy,
  - halogenated C<sub>1</sub>-C<sub>7</sub> alkoxy,
  - C<sub>1</sub>-C<sub>7</sub> alkoxy substituted by carbocyclic aryl,
  - methylcarbonyloxy,
  - carbocyclic aryloxy,
  - carbocyclic aryloxy substituted by methoxy,
  - amino,
  - di-methylamino,
  - propargynylcarbonylamino substituted by carbocyclic aryl,
  - carbocyclic arylsulfonylamino substituted by methyl,
  - (carbocyclic aryl)NHC(O)NH substituted by halogenated methoxy,
  - halogenated methylthio,
  - carbocyclic arylthio substituted by cyano,
  - di-propylamino sulfonyl,
  - mono- or di- ethylaminocarbonyl substituted by carbocyclic aryl,
  - carbocyclic aryl,
  - heterocyclyl substituted by methyl,
  - heterocyclyl substituted by halogenated carbocyclic aryl,
- (vi) heterocyclyl,  
or heterocyclyl substituted by substituent(s) independently selected from
  - halogen,
  - nitro,
  - C<sub>1</sub>-C<sub>4</sub> alkyl,

- C<sub>1</sub>-C<sub>4</sub> alkyl substituted by substituent(s) independently selected from
  - halogen,
  - methylthio substituted by halogenated carbocyclic aryl,
  - carbocyclic aryl,
  - halogenated carbocyclic aryl,
  - heterocyclyl,
  - methoxy,
  - carbocyclic aryloxy,
  - carbocyclic aryloxy substituted by methyl,
  - C<sub>1</sub>-C<sub>3</sub> alkylthio,
  - propenylthio,
  - carbocyclic arylthio,
  - C<sub>1</sub>-C<sub>3</sub> alkylsulfonyl,
  - carbocyclic arylsulfonyl substituted by C<sub>1</sub>-C<sub>4</sub> alkyl,
  - carbocyclic aryl,
  - halogenated carbocyclic aryl,
  - carbocyclic aryl substituted by methyl,
  - carbocyclic aryl substituted by nitro,
  - heterocyclyl;

R<sub>2</sub> is methylamino or dimethylamino;

L is selected from Formula Va, VIIIa, or IXa;

wherein R<sub>4</sub> and R<sub>5</sub> are independently selected from H or C<sub>1</sub>-C<sub>3</sub> alkyl;

wherein carbocyclic aryl is phenyl, naphthyl, anthranyl, or biphenyl;

carbocyclyl is 1-oxo-indanyl, 9-oxo-fluorenyl, indenyl, anthraquinonyl, C-fluoren-9-ylidene, 1,2,3,4-tetrahydro-naphthyl, or bicyclo[2.2.1]hepteny;

heterocyclyl is 1,2,3-thiadiazolyl, 1,2,3-triazolyl, 1,2-dihydro-3-oxo-pyrazolyl, 1,3-dioxo-isoindolyl, 1*H*-indolyl, 1*H*-pyrrolyl, 1-oxo-3*H*-isobenzofuranyl, 2,3-dihydro-benzo[1,4]dioxinyl, 2,4-dihydro-3-oxo-pyrazolyl, 2*H*-benzopyranyl, 2-oxo-benzopyranyl, 3,4-dihydro-2*H*-benzo[b][1,4]dioxepinyl, 4-oxo-3,4-dihydro-phthalazinyl, 4-oxo-benzopyranyl, 9,10,10-trioxo-thioxanthenyl, 9*H*-xanthenyl, azetidiny, benzimidazolyl, benzo[1,3]dioxolyl, benzo[2,1,3]oxadiazolyl, benzo[b]thienyl, furyl, imidazolyl, isoxazolyl, morpholino, morpholinyl, oxolanyl, piperidyl, piridyl, pyrazolyl, pyridyl, quinolyl,

quinoxalyl, thiazolidyl, thiazolyl, thienyl, thiolanyl, 2,3-dihydro-1-oxo-isindolyl, 2,3-dihydro-benzofuryl, 2-oxo-pyrrolidinyl, 4-oxo-1,5,6,7-tetrahydro-indolyl, cinnolyl, pyrimidyl, pyrrolidyl, tetrahydro-thienyl, benzofuranyl, or benzothiazolyl;

halogen is fluoro, chloro, bromo, or iodo;  
or a salt thereof.

4. A compound according to claim 3, wherein

R<sub>1</sub> represents

(i) C<sub>1</sub>-C<sub>10</sub> alkyl substituted by substituent(s) independently selected from

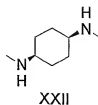
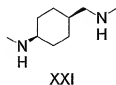
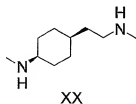
- oxo,
- di-propylaminocarbonyl,
- methoxy substituted by carbocyclic aryl,
- methylcarbonyloxy,
- carbocyclic aryloxy,
- halogenated carbocyclic aryloxy,
- carbocyclic aryloxy substituted by nitro,
- heterocycloxy substituted by methyl,
- substituted heterocyclyl-ethylideneaminoxy,
- tert*-butoxycarbonylamino,
- carbocyclic arylcarbonylamino,
- C<sub>1</sub>-C<sub>2</sub> alkylthio,
- C<sub>1</sub>-C<sub>2</sub> alkylthio substituted by substituent(s) independently selected from
  - halogenated carbocyclic aryl,
  - carbocyclic aryl substituted by methoxy,
  - carbocyclic arylthio,
  - heterocyclylthio substituted by nitro,
  - heterocyclylthio substituted by methyl,
  - C<sub>5</sub>-C<sub>6</sub> cycloalkenyl,
  - carbocyclyl substituted by substituent(s) independently selected from
    - halogen,
    - methyl,
    - methoxy,

- ethenyl substituted by carbocyclic aryl substituted methylsulfinyl,
- carbocyclic aryl substituted by substituent(s) independently selected from
  - halogen,
  - hydroxy,
  - nitro,
  - C<sub>1</sub>-C<sub>4</sub> alkyl,
  - C<sub>1</sub>-C<sub>4</sub> alkyl substituted by substituent(s) independently selected from
    - OXO,
    - carbocyclic aryl,
    - heterocyclyl,
    - C<sub>1</sub>-C<sub>4</sub> alkoxy,
    - halogenated C<sub>1</sub>-C<sub>4</sub> alkoxy,
    - C<sub>1</sub>-C<sub>4</sub> alkoxy substituted by carbocyclic aryl,
    - carbocyclic aryloxy,
    - halogenated mono-carbocyclic arylaminocarbonyl,
    - carbocyclic aryl,
    - heterocyclyl,
    - heterocyclyl substituted by substituent(s) independently selected from
      - C<sub>1</sub>-C<sub>2</sub> alkyl,
      - C<sub>1</sub>-C<sub>2</sub> substituted by carbocyclic aryl,
      - methoxy,
      - methoxy substituted by carbocyclic aryl,
      - carbocyclic aryl,
      - halogenated carbocyclic aryl,
- (ii) C<sub>2</sub>-C<sub>3</sub> alkenyl substituted by substituent(s) independently selected from
  - carbocyclic aryl,
  - halogenated carbocyclic aryl,
  - carbocyclic aryl substituted by nitro,
- (iii) C<sub>3</sub>-C<sub>6</sub> cycloalkyl substituted by substituent(s) independently selected from
  - methyl substituted by oxo,
  - methyl substituted by carbocyclic aryl,
  - carbocyclic aryl,

- (iv) carbocyclcyl,
- (v) carbocyclic aryl substituted by substituent(s) independently selected from
  - halogen,
  - hydroxy,
  - cyano,
  - nitro,
  - C<sub>1</sub>-C<sub>9</sub> alkyl,
  - C<sub>1</sub>-C<sub>9</sub> alkyl substituted by substituent(s) independently selected from
    - halogen,
    - oxo,
    - carbocyclic aryl,
    - carbocyclic aryl substituted by methyl,
    - carbocyclic aryloxy,
    - C<sub>1</sub>-C<sub>7</sub> alkoxy,
    - halogenated C<sub>1</sub>-C<sub>7</sub> alkoxy,
    - C<sub>1</sub>-C<sub>7</sub> alkoxy substituted by carbocyclic aryl,
    - methylcarbonyloxy,
    - carbocyclic aryloxy,
    - carbocyclic aryloxy substituted by methoxy,
    - amino,
    - di-methylamino,
    - propargynylcarbonylamino substituted by carbocyclic aryl,
    - carbocyclic arylsulfonylamino substituted by methyl,
    - (carbocyclic aryl)NHC(O)NH substituted by halogenated methoxy,
    - halogenated methylthio,
    - carbocyclic arylthio substituted by cyano,
    - di-propylamino sulfonyl,
    - mono- or di- ethylaminocarbonyl substituted by carbocyclic aryl,
    - carbocyclic aryl,
    - heterocyclcyl substituted by methyl,
    - heterocyclcyl substituted by halogenated carbocyclic aryl,
- (vi) or heterocyclcyl substituted by substituent(s) independently selected from

- halogen,
- nitro,
- C<sub>1</sub>-C<sub>4</sub> alkyl,
- C<sub>1</sub>-C<sub>4</sub> alkyl substituted by substituent(s) independently selected from
  - halogen,
  - methylthio substituted by halogenated carbocyclic aryl,
  - carbocyclic aryl,
  - halogenated carbocyclic aryl,
  - heterocyclyl,
  - methoxy,
  - carbocyclic aryloxy,
  - carbocyclic aryloxy substituted by methyl,
  - C<sub>1</sub>-C<sub>3</sub> alkylthio,
  - propenylthio,
  - carbocyclic arylthio,
  - C<sub>1</sub>-C<sub>3</sub> alkylsulfonyl,
  - carbocyclic arylsulfonyl,
  - carbocyclic arylsulfonyl substituted by C<sub>1</sub>-C<sub>4</sub> alkyl,
  - carbocyclic aryl,
  - halogenated carbocyclic aryl,
  - carbocyclic aryl substituted by methyl,
  - carbocyclic aryl substituted by nitro,
  - heterocyclyl;

L is selected from Formula XX - XXII;



wherein carbocyclic aryl is phenyl, naphthyl, or biphenyl;

carbocyclyl is 1-oxo-indanyl, 9-oxo-fluorenyl, indenyl, anthraquinonyl, C-fluoren-

9-ylidene, 1,2,3,4-tetrahydro-naphthyl, or bicyclo[2.2.1]hepteny;

heterocyclyl is 1,2,3-thiadiazolyl, 1,2,3-triazolyl, 1,2-dihydro-3-oxo-pyrazolyl, 1*H*-indolyl, 1*H*-pyrrolyl, 2,4-dihydro-3-oxo-pyrazolyl, 2*H*-benzopyranyl, 4-oxo-benzopyranyl, azetidiny, benzo[b]thienyl, furyl, isoxazolyl, morpholinyl, piperidyl, piridyl, pyrazolyl, pyridyl, quinolyl, thiazolidyl, thiazolyl, thienyl, thiolanyl, 2,3-dihydro-1-oxo-isindolyl, 2,3-dihydro-benzofuryl, 2-oxo-benzopyranyl, 2-oxo-pyrrolidinyl, 4-oxo-1,5,6,7-tetrahydro-indolyl, 9*H*-xanthenyl, cinnolyl, imidazolyl, morpholino, pyrimidyl, pyrrolidyl, tetrahydro-thienyl, benzofuranyl, or benzothiazolyl;

halogen is fluoro, chloro, bromo, or iodo;

or a salt thereof.

5. A compound according to claim 4, wherein

R<sub>1</sub> represents

(i) C<sub>1</sub>-C<sub>5</sub> alkyl substituted by substituent(s) independently selected from

- oxo,
- di-propylaminocarbonyl,
- methoxy substituted by carbocyclic aryl,
- methylcarbonyloxy,
- carbocyclic aryloxy,
- halogenated carbocyclic aryloxy,
- carbocyclic aryloxy substituted by nitro,
- heterocyclyloxy substituted by methyl,
- substituted heterocyclyl-ethylideneaminoxy,
- tert*-butoxycarbonylamino,
- carbocyclic arylcarbonylamino,
- C<sub>1</sub>-C<sub>2</sub> alkylthio,
- C<sub>1</sub>-C<sub>2</sub> alkylthio substituted by substituent(s) independently selected from
- halogenated carbocyclic aryl,
- carbocyclic aryl substituted by methoxy,
- carbocyclic arylthio,
- heterocyclylthio substituted by nitro,
- heterocyclylthio substituted by methyl,



- cyclohexenyl,
- carbocyclyl substituted by substituent(s) independently selected from
  - halogen,
  - methyl,
  - methoxy,
  - ethenyl substituted by carbocyclic aryl substituted methylsulfinyl,
  - carbocyclic aryl substituted by substituent(s) independently selected from
    - halogen,
    - hydroxy,
    - nitro,
    - C<sub>1</sub>-C<sub>4</sub> alkyl,
    - C<sub>1</sub>-C<sub>4</sub> alkyl substituted by substituent(s) independently selected from
      - oxo,
      - carbocyclic aryl,
      - heterocyclyl,
      - C<sub>1</sub>-C<sub>2</sub> alkoxy,
      - halogenated C<sub>1</sub>-C<sub>2</sub> alkoxy,
      - C<sub>1</sub>-C<sub>2</sub> alkoxy substituted by carbocyclic aryl,
      - carbocyclic aryloxy,
      - halogenated mono-carbocyclic arylaminocarbonyl,
      - carbocyclic aryl,
      - heterocyclyl,
      - heterocyclyl substituted by substituent(s) independently selected from
        - C<sub>1</sub>-C<sub>2</sub> alkyl,
        - C<sub>1</sub>-C<sub>2</sub> substituted by carbocyclic aryl,
        - methoxy,
        - methoxy substituted by carbocyclic aryl,
        - carbocyclic aryl,
        - halogenated carbocyclic aryl,
- (ii) C<sub>2</sub>-C<sub>3</sub> alkenyl substituted by substituent(s) independently selected from
  - carbocyclic aryl,
  - halogenated carbocyclic aryl,

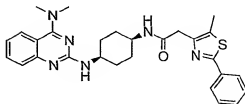
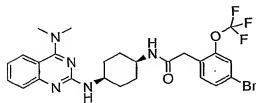
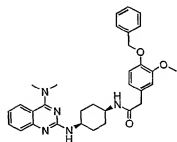
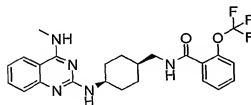
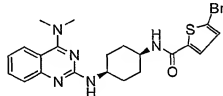
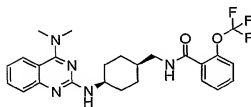
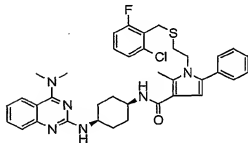
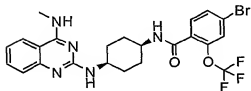
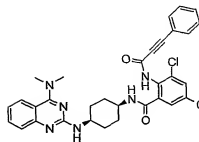
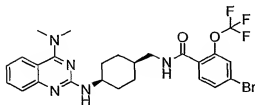
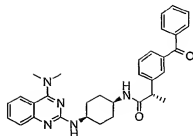
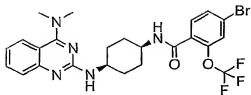
- carbocyclic aryl substituted by nitro,
- (iii) C<sub>3</sub>-C<sub>6</sub> cycloalkyl substituted by substituent(s) independently selected from
  - methyl substituted by oxo,
  - methyl substituted by carbocyclic aryl,
  - carbocyclic aryl,
- (iv) carbocyclyl,
- (v) carbocyclic aryl substituted by substituent(s) independently selected from
  - halogen,
  - hydroxy,
  - cyano,
  - nitro,
  - C<sub>1</sub>-C<sub>4</sub> alkyl,
  - C<sub>1</sub>-C<sub>2</sub> alkyl substituted by substituent(s) independently selected from
    - halogen,
    - oxo,
    - carbocyclic aryl,
    - carbocyclic aryl substituted by methyl,
    - carbocyclic aryloxy,
    - C<sub>1</sub>-C<sub>2</sub> alkoxy,
    - halogenated C<sub>1</sub>-C<sub>2</sub> alkoxy,
    - C<sub>1</sub>-C<sub>2</sub> alkoxy substituted by carbocyclic aryl,
    - methylcarbonyloxy,
    - carbocyclic aryloxy,
    - carbocyclic aryloxy substituted by methoxy,
    - amino,
    - di-methylamino,
    - propargynylcarbonylamino substituted by carbocyclic aryl,
    - carbocyclic arylsulfonylamino substituted by methyl,
    - (carbocyclic aryl)NHC(O)NH substituted by halogenated methoxy,
    - halogenated methylthio,
    - carbocyclic arylthio substituted by cyano,
    - di-propylamino sulfonyl,

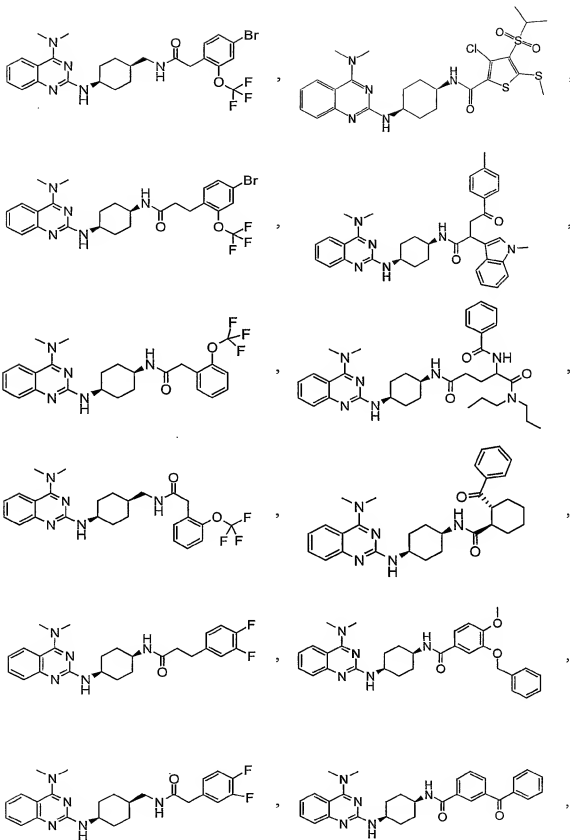
- mono- or di- ethylaminocarbonyl substituted by carbocyclic aryl,
- carbocyclic aryl,
- heterocyclyl substituted by methyl,
- heterocyclyl substituted by halogenated carbocyclic aryl,
- (vi) or heterocyclyl substituted by substituent(s) independently selected from
  - halogen,
  - nitro,
  - C<sub>1</sub>-C<sub>4</sub> alkyl,
  - C<sub>1</sub>-C<sub>4</sub> alkyl substituted by substituent(s) independently selected from
    - halogen,
    - methylthio substituted by halogenated carbocyclic aryl,
    - carbocyclic aryl,
    - halogenated carbocyclic aryl,
    - heterocyclyl,
    - methoxy,
    - carbocyclic aryloxy,
    - carbocyclic aryloxy substituted by methyl,
    - C<sub>1</sub>-C<sub>3</sub> alkylthio,
    - propenylthio,
    - carbocyclic arylthio,
    - C<sub>1</sub>-C<sub>3</sub> alkylsulfonyl,
    - carbocyclic arylsulfonyl,
    - carbocyclic arylsulfonyl substituted by methyl,
    - carbocyclic aryl,
    - halogenated carbocyclic aryl,
    - carbocyclic aryl substituted by methyl,
    - carbocyclic aryl substituted by nitro,
    - heterocyclyl;
      - wherein carbocyclic aryl is phenyl , naphthyl, or biphenyl;
      - carbocyclyl is 1-oxo-indanyl, indenyl, 9-oxo-fluorenyl, 1,2,3,4-tetrahydro-naphthyl,
      - or bicyclo[2.2.1]hepteny;
      - heterocyclyl is 1*H*-indolyl, 2,4-dihydro-3-oxo-pyrazolyl, furyl, pyrazolyl, pyridyl,

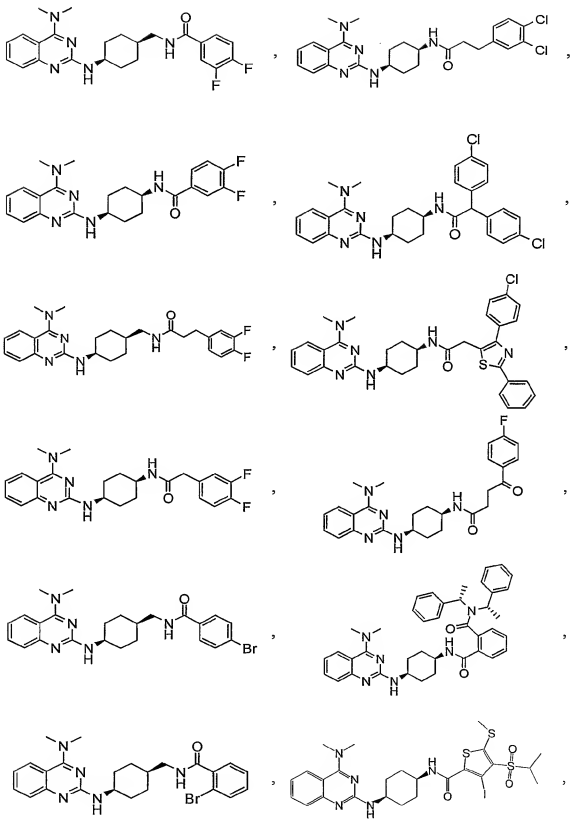
thienyl, 1,2,3-triazolyl, 1*H*-pyrrolyl, 2,3-dihydro-1-oxo-isoindolyl, 2,3-dihydro-benzofuryl, 2*H*-benzopyranyl, 2-oxo-benzopyranyl, 4-oxo-1,5,6,7-tetrahydro-indolyl, imidazolyl, isoxazolyl, morpholino, morpholinyl, pyrazolyl, pyrimidyl, quinolyl, thiazolyl, tetrahydro-thienyl, benzofuranyl, or benzothiazolyl;

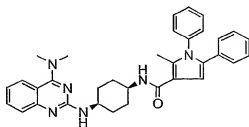
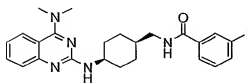
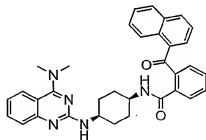
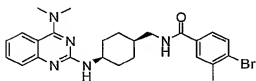
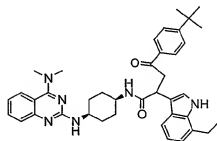
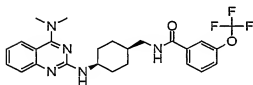
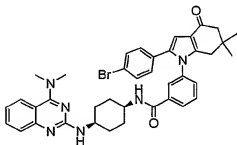
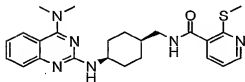
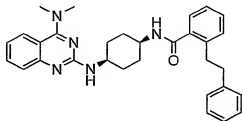
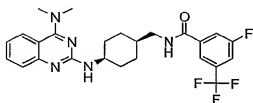
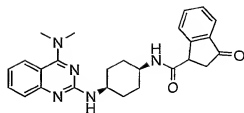
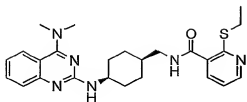
halogen is fluoro, chloro, bromo, or iodo;  
or a salt thereof.

6. A compound according to claim 5 of Formua I selected from the group consisting of

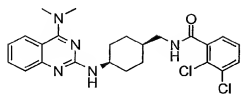




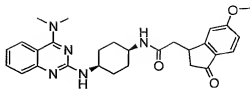




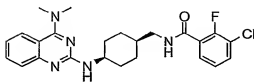




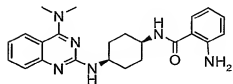
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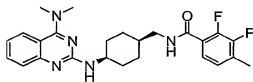
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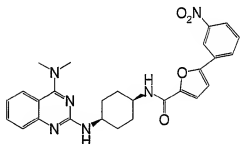
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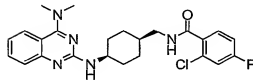
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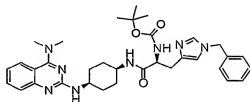
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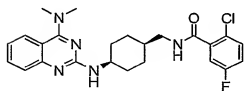
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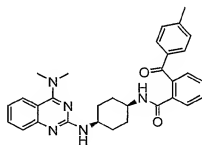
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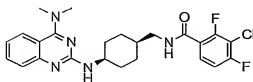
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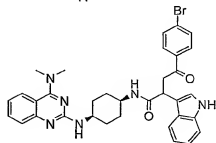
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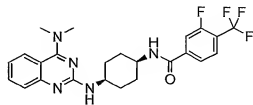
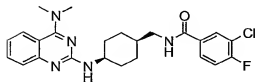
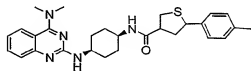
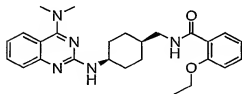
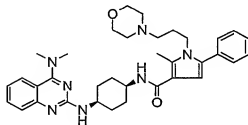
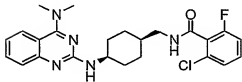
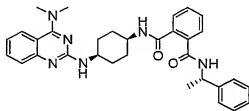
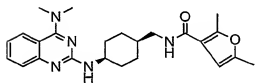
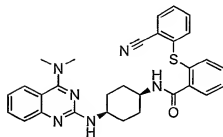
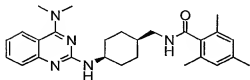
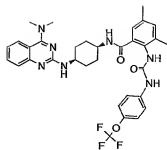
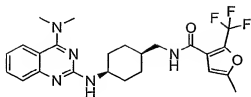
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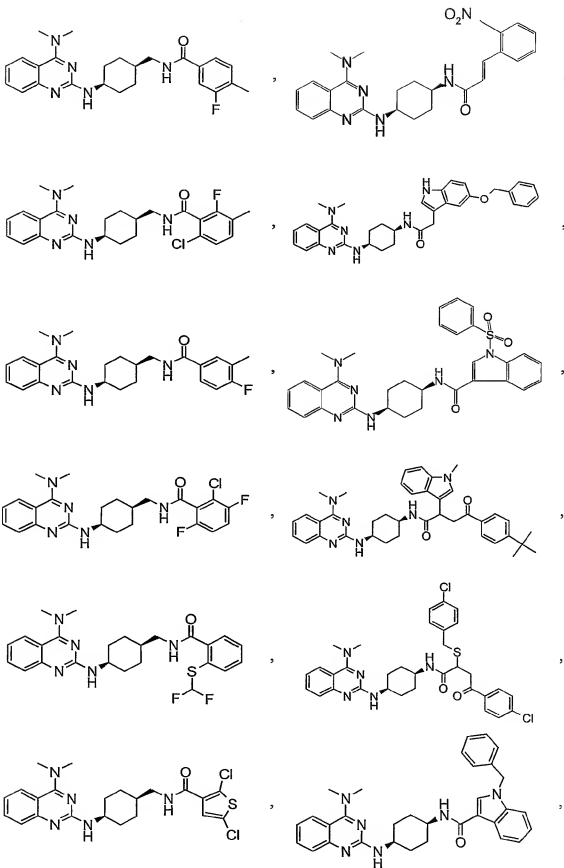


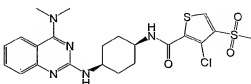
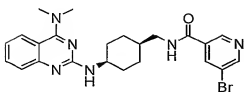
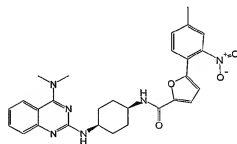
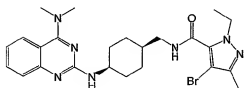
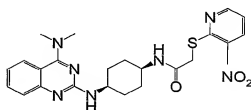
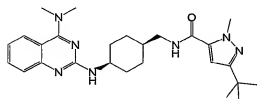
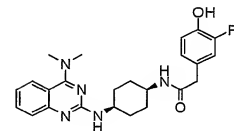
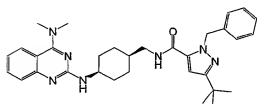
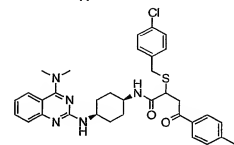
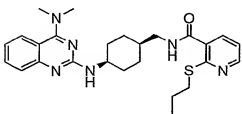
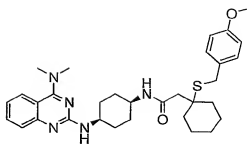
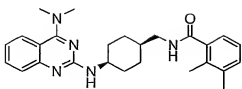
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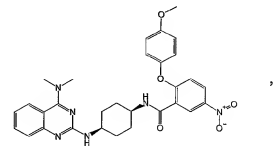
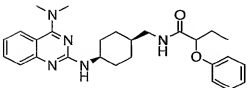
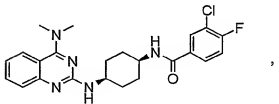
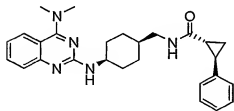
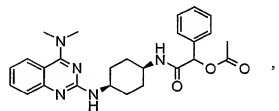
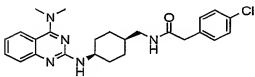
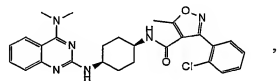
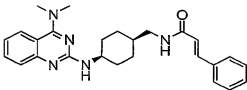
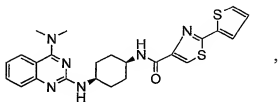
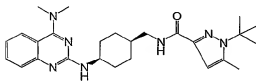
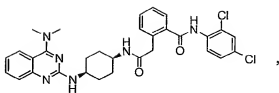
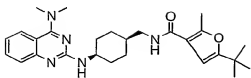


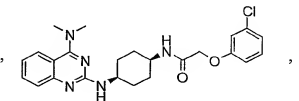
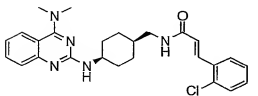
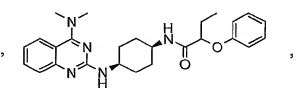
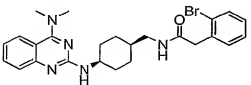
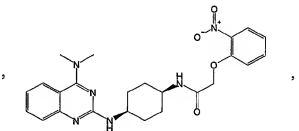
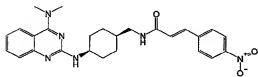
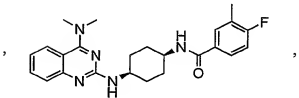
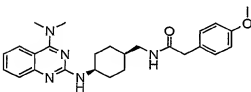
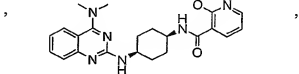
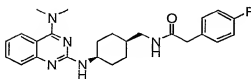
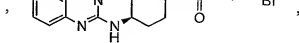
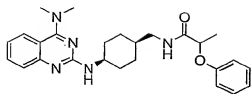
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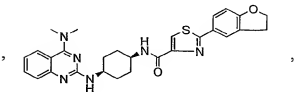
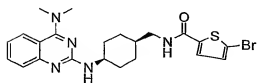
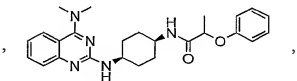
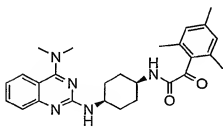
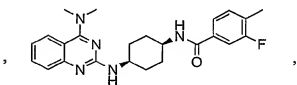
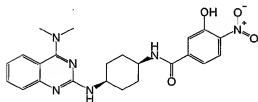
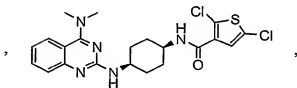
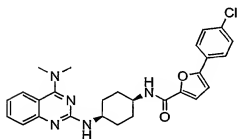
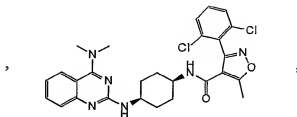
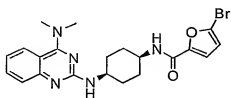
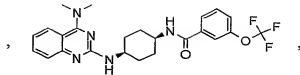
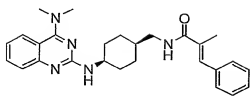


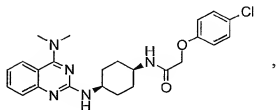
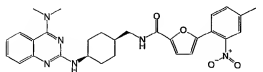
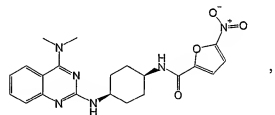
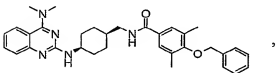
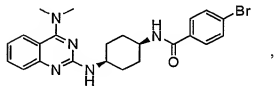
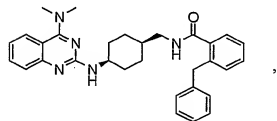
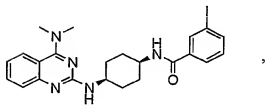
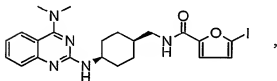
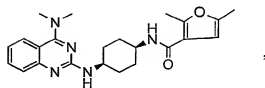
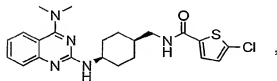
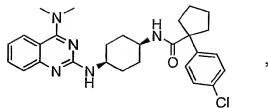
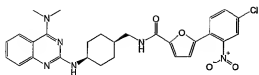




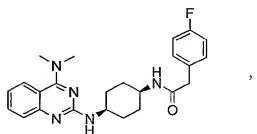
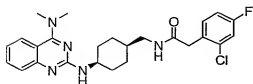
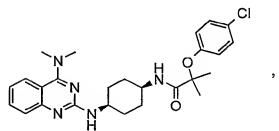
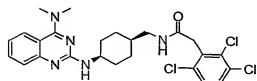
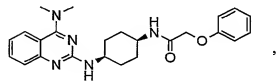
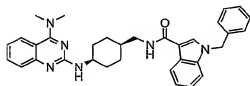
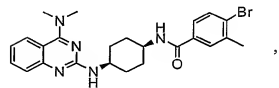
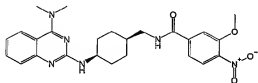
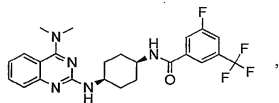
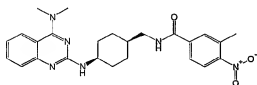
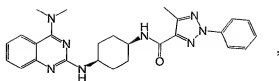
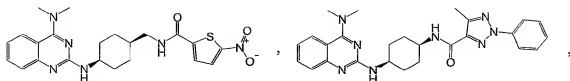


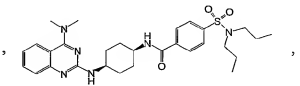
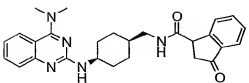
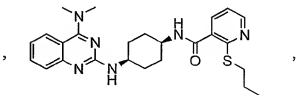
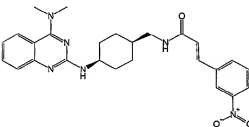
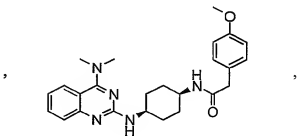
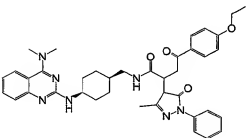
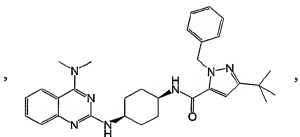
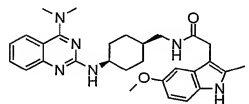
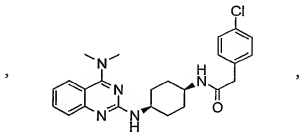
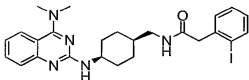
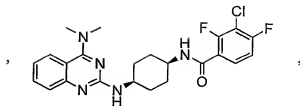
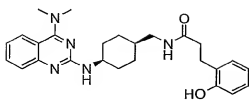


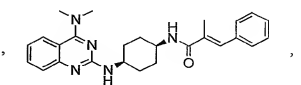
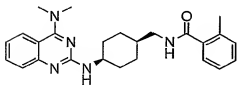
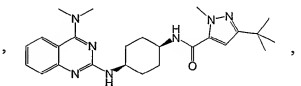
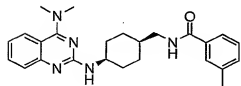
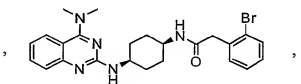
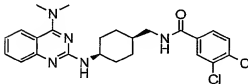
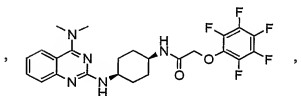
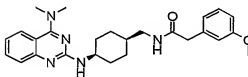
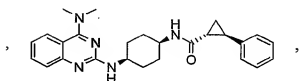
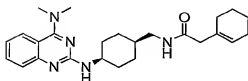
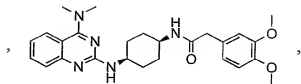
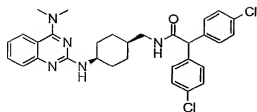


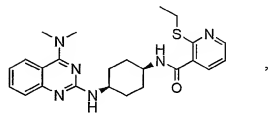
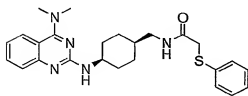
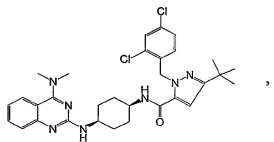
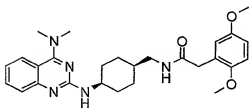
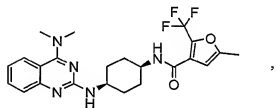
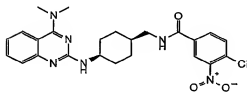
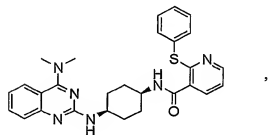
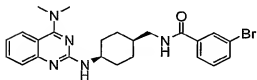
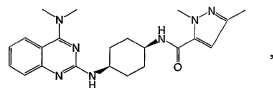
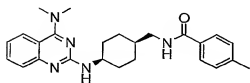
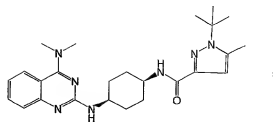
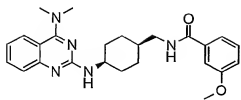




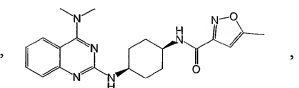
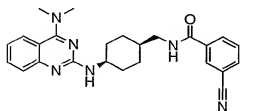
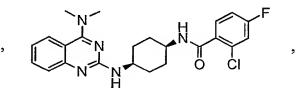
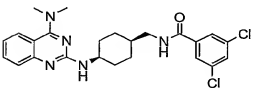
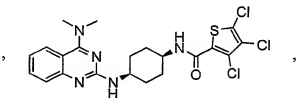
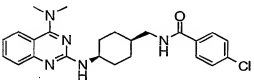
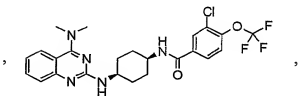
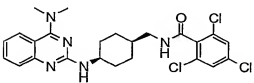
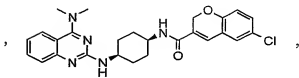
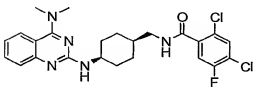
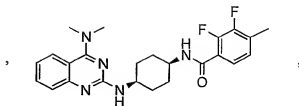
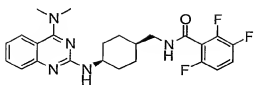


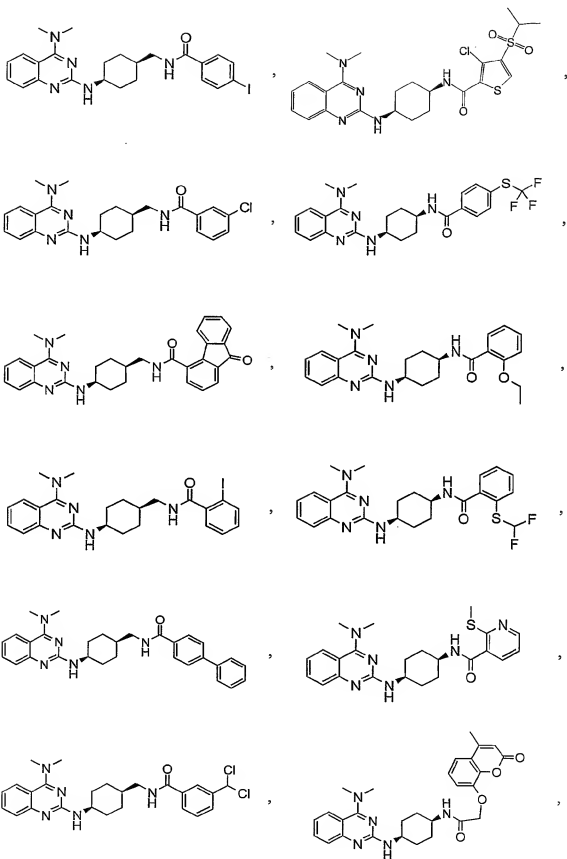


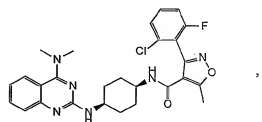
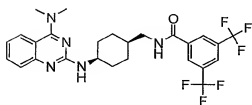
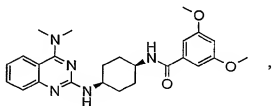
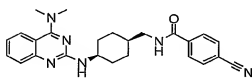
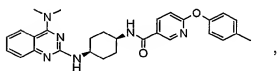
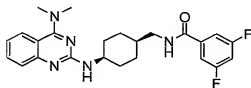
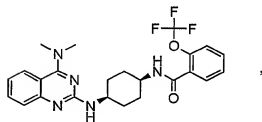
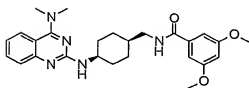
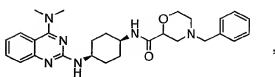
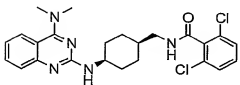
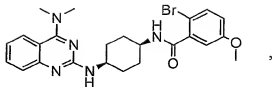
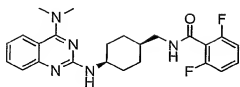




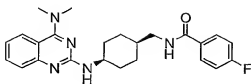




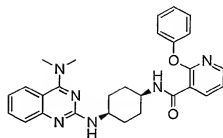




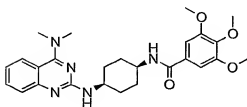




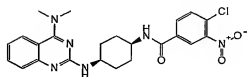
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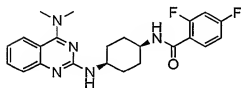
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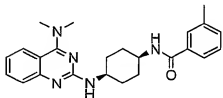
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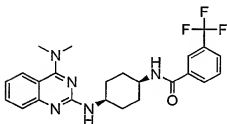
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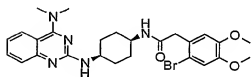
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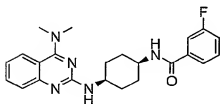
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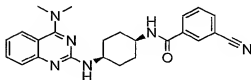
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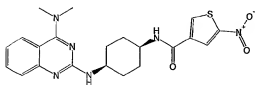
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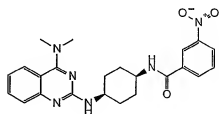
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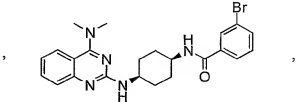
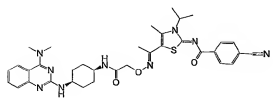
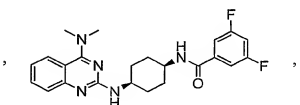
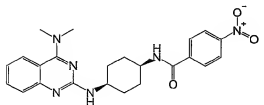
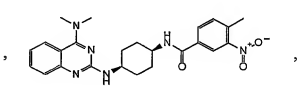
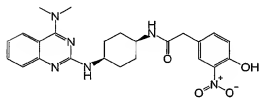
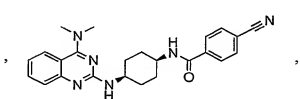
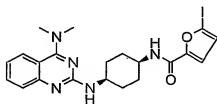
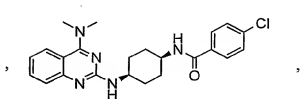
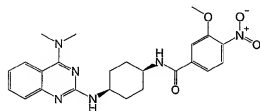
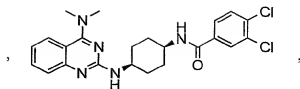
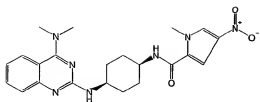
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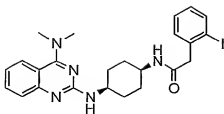


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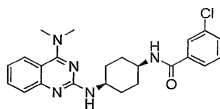


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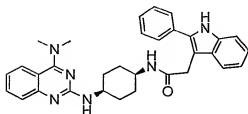




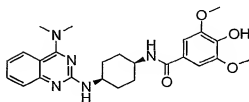
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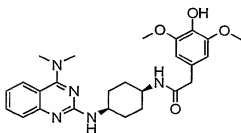
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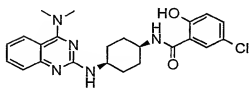
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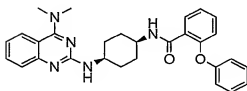
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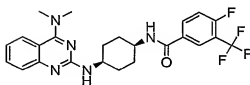
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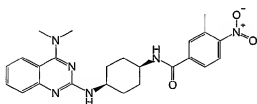
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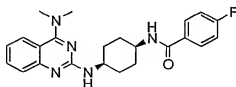
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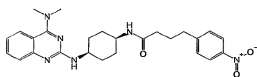
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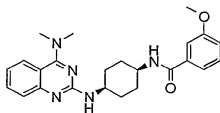
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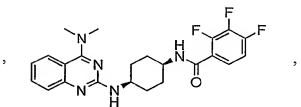
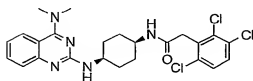
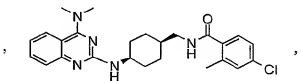
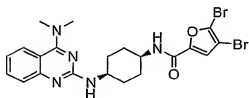
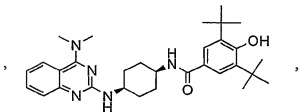
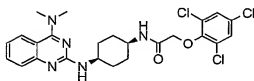
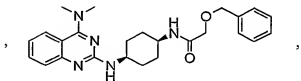
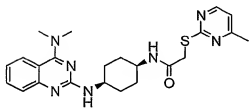
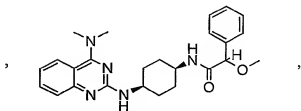
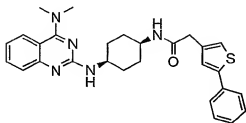
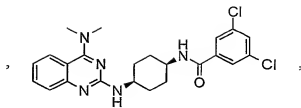
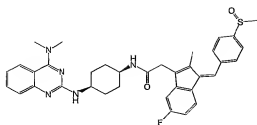
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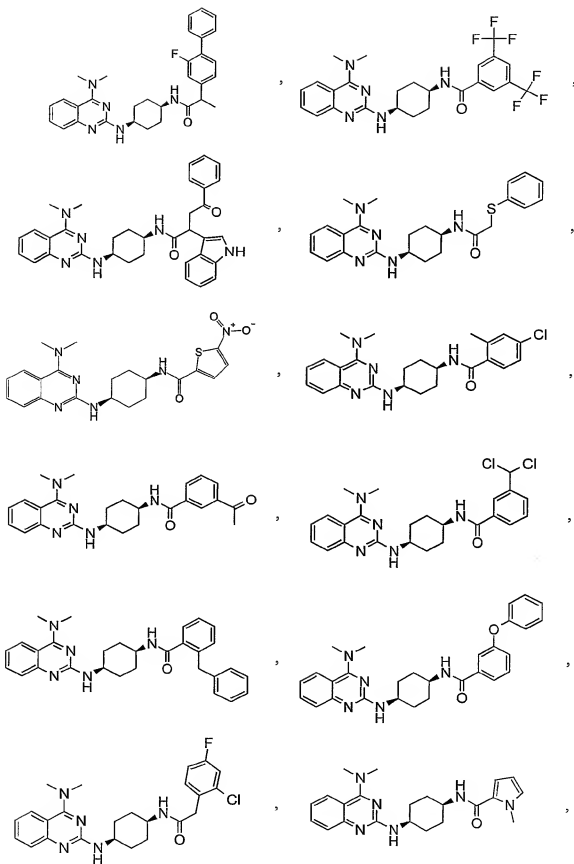


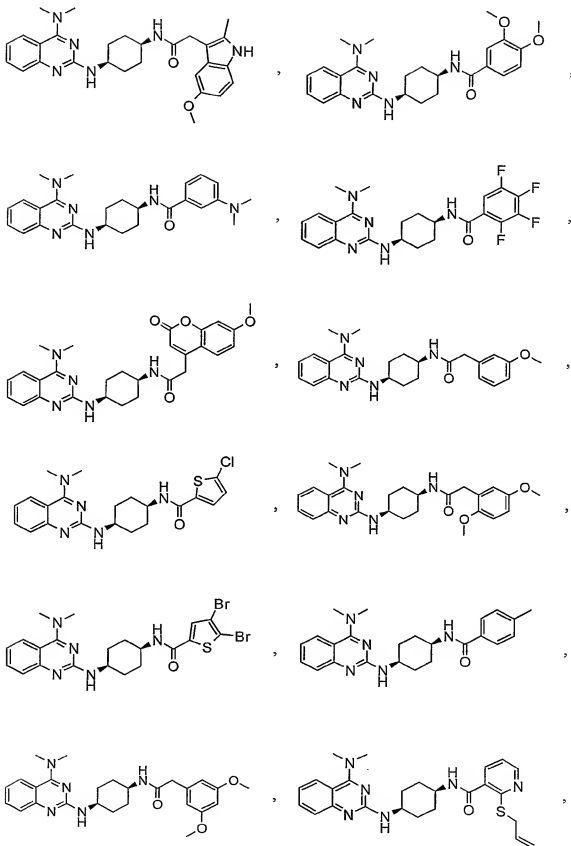
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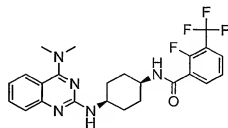
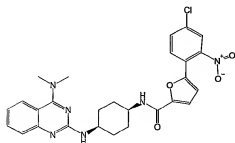
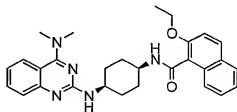
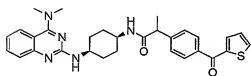
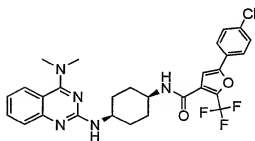
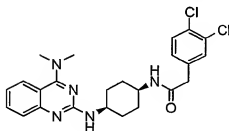
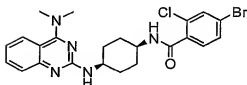
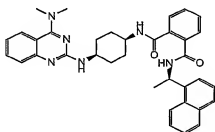
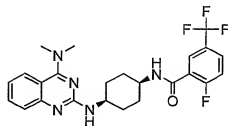
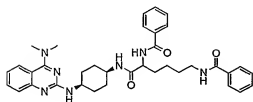
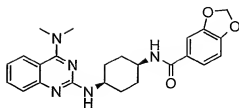
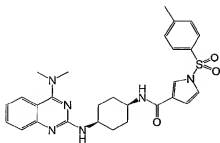


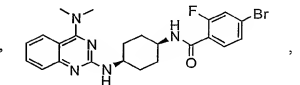
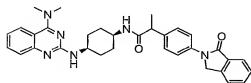
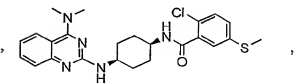
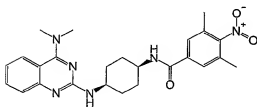
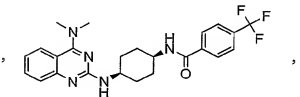
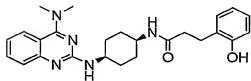
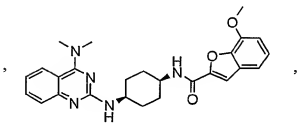
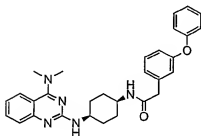
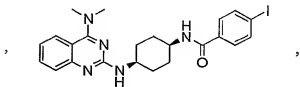
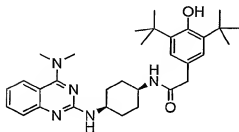
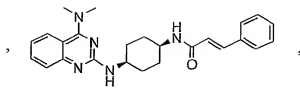
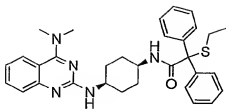
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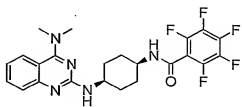
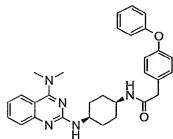
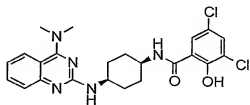
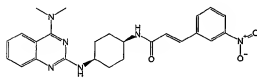
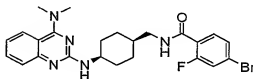
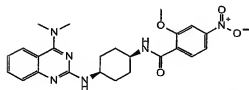
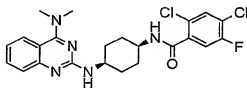
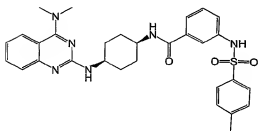
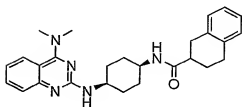
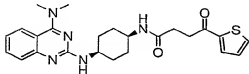
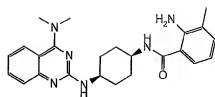
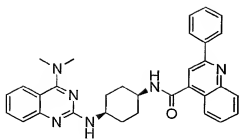


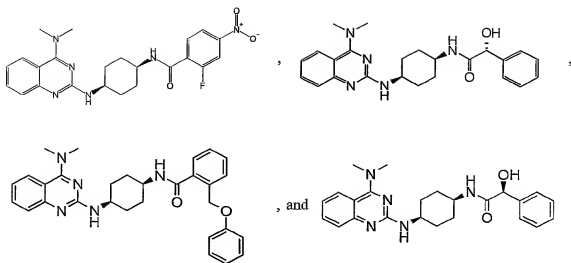












; or, in case of, a salt thereof.

7. A compound according to claim 3, wherein

R<sub>1</sub> represents

(i) C<sub>1</sub>-C<sub>10</sub> alkyl,

C<sub>1</sub>-C<sub>10</sub> alkyl substituted by substituent(s) independently selected from

•C<sub>3</sub>-C<sub>6</sub> cycloalkyl,

•carbocyclic aryl,

•heterocyclyl,

(ii) C<sub>3</sub>-C<sub>6</sub> cycloalkyl,

(iii) carbocyclic aryl,

(iv) or heterocyclyl;

L is selected from Formula XX - XXII;

wherein carbocyclic aryl is phenyl, naphthyl, anthranyl, or biphenyl;

heterocyclyl is 1,3-dioxo-isindolyl, 1*H*-indolyl, 1-oxo-3*H*-isobenzofuranyl, 2,3-dihydro-benzo[1,4]dioxinyl, 3,4-dihydro-2*H*-benzo[b][1,4]dioxepinyl, 4-oxo-3,4-dihydro-phthalazinyl, 9,10,10-trioxo-thioxanthenyl, 9*H*-xanthenyl, benzimidazolyl, benzo[1,3]dioxolyl, benzo[2,1,3]oxadiazolyl, benzo[b]thienyl, furyl, imidazolyl, isoxazolyl, morpholino, oxolanyl, piperidyl, pyridyl, quinoxalyl, thienyl, quinolyl, or benzothiazolyl; or a salt thereof.

8. A compound according to claim 7, wherein

R<sub>1</sub> represents

(i) C<sub>1</sub>-C<sub>4</sub> alkyl,

C<sub>1</sub>-C<sub>4</sub> alkyl substituted by substituent(s) independently selected from

•cyclopentyl,

•carbocyclic aryl,

•heterocyclyl,

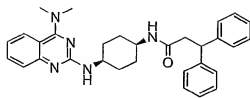
(ii) carbocyclic aryl,

(iii) or heterocyclyl;

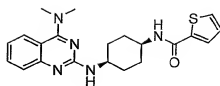
wherein carbocyclic aryl is phenyl, naphthyl, anthranyl, or biphenyl;

heterocyclyl is 9*H*-xanthenyl, benzo[1,3]dioxolyl, benzo[2,1,3]oxadiazolyl, benzo[b]thienyl, thienyl, 1*H*-indolyl, quinoxalyl, quinolyl, or benzothiazolyl; or a salt thereof.

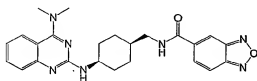
9. A compound according to claim 8 of Formula I thereof selected from the group consisting of



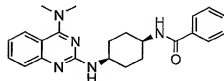
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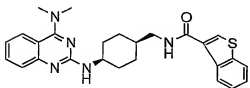
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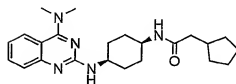
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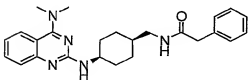
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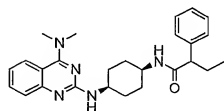
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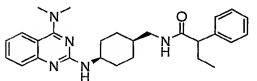
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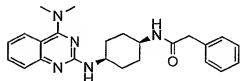
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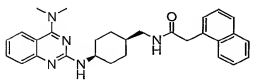
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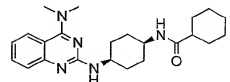
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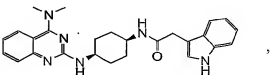
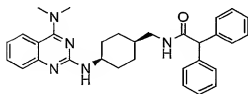
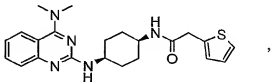
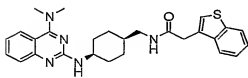
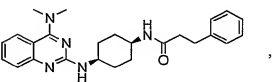
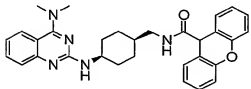
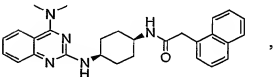
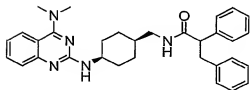
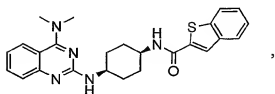
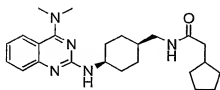
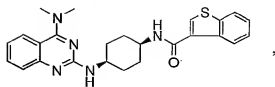
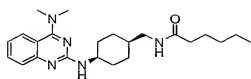
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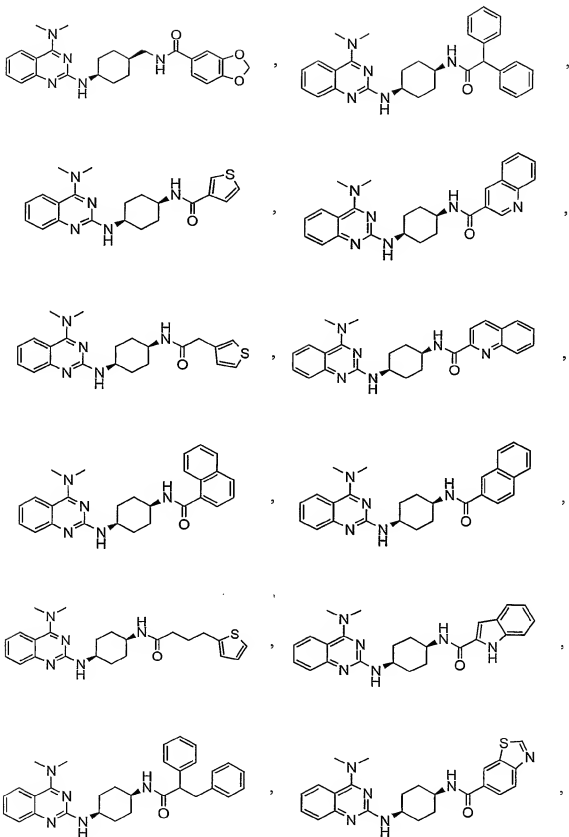


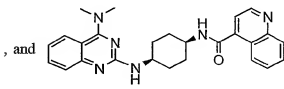
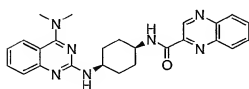
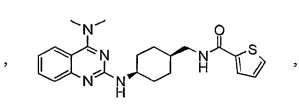
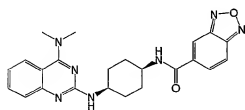
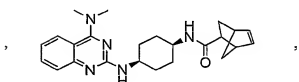
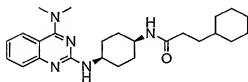
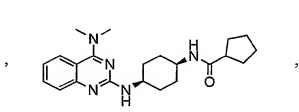
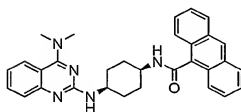
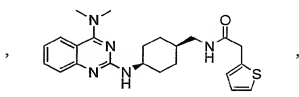
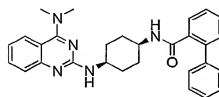
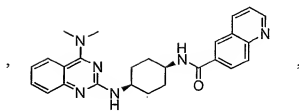
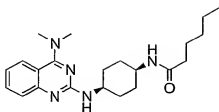
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, and

; or, in case of, a salt thereof.



10. A compound according to claim 1, wherein Q is Formula II;

R<sub>1</sub> represents

- (i) C<sub>1</sub>-C<sub>10</sub> alkyl,
- C<sub>1</sub>-C<sub>10</sub> alkyl substituted by substituent(s) independently selected from
  - halogen,
  - hydroxy,
  - oxo,
  - C<sub>1</sub>-C<sub>3</sub> alkoxy,
  - C<sub>1</sub>-C<sub>3</sub> alkoxy substituted by substituent(s) independently selected from
    - carbocyclic aryl,
    - heterocyclyl,
    - heterocyclyl substituted by C<sub>1</sub>-C<sub>3</sub> alkyl,
    - carbocyclic aryloxy,
    - carbocyclic aryloxy substituted by substituent(s) independently selected from
      - halogen,
      - nitro,
      - carbocyclic aryl,
      - carbocyclic aryl substituted by C<sub>1</sub>-C<sub>3</sub> alkoxy,
      - C<sub>1</sub>-C<sub>4</sub> alkyl,
      - C<sub>1</sub>-C<sub>4</sub> alkyl substituted by substituent(s) independently selected from
        - mono- or di-C<sub>1</sub>-C<sub>3</sub> alkylamino,
        - mono- or di-C<sub>1</sub>-C<sub>3</sub> alkylamino substituted by carbocyclic aryl,
        - mono- or di-C<sub>1</sub>-C<sub>3</sub> alkylamino substituted by halogenated carbocyclic aryl,
        - mono- or di-C<sub>1</sub>-C<sub>3</sub> alkylamino,
        - mono- or di-C<sub>1</sub>-C<sub>3</sub> alkylamino substituted by substituent(s) independently selected from
          - cyano,
          - carbocyclic aryl,
          - heterocyclyl,
          - mono- or di-carbocyclic arylamino,
          - mono- or di-carbocyclic arylamino substituted by C<sub>1</sub>-C<sub>3</sub> alkyl,
          - C<sub>1</sub>-C<sub>3</sub> alkylcarbonylamino,
          - C<sub>1</sub>-C<sub>4</sub> alkoxycarbonylamino,

- carbocyclic arylsulfonylamino,
- carbocyclic arylsulfonylamino substituted by substituent(s) independently selected from
  - nitro,
  - C<sub>1</sub>-C<sub>3</sub> alkyl,
  - mono- or di-C<sub>1</sub>-C<sub>3</sub> alkylamino,
  - C<sub>1</sub>-C<sub>3</sub> alkylthio,
  - C<sub>1</sub>-C<sub>3</sub> alkylthio substituted by substituent(s) independently selected from
    - mono- or di-carbocyclic arylamino,
    - halogenated mono- or di-carbocyclic arylamino,
    - carbocyclic aryl,
    - carbocyclic aryl substituted by substituent(s) independently selected from
      - halogen,
      - C<sub>1</sub>-C<sub>3</sub> alkoxy,
    - carbocyclic arylthio,
    - carbocyclic arylthio substituted by substituent(s) independently selected from
      - halogen,
      - C<sub>1</sub>-C<sub>3</sub> alkyl,
    - carbocyclic arylsulfonyl,
    - halogenated carbocyclic arylsulfonyl,
    - heterocyclylthio,
    - C<sub>3</sub>-C<sub>6</sub> cycloalkyl,
    - C<sub>3</sub>-C<sub>6</sub> cycloalkyl substituted by C<sub>1</sub>-C<sub>3</sub> alkyl,
    - carbocyclyl,
    - carbocyclyl substituted by substituent(s) independently selected from
      - halogen,
      - C<sub>1</sub>-C<sub>3</sub> alkyl,
      - C<sub>2</sub>-C<sub>3</sub> alkenyl,
      - C<sub>2</sub>-C<sub>3</sub> alkenyl substituted by carbocyclic aryl,
      - C<sub>2</sub>-C<sub>3</sub> alkenyl substituted by carbocyclic aryl substituted C<sub>1</sub>-C<sub>3</sub> alkylsulfinyl,
    - carbocyclic aryl,
    - carbocyclic aryl substituted by substituent(s) independently selected from
      - halogen,

- hydroxy,
- nitro,
- C<sub>1</sub>-C<sub>4</sub> alkyl,
- C<sub>1</sub>-C<sub>4</sub> alkyl substituted by substituent(s) independently selected from
  - halogen,
  - hydroxy,
  - carbocyclic aryl,
  - mono- or di-carbocyclic arylamino,
  - mono- or di-carbocyclic arylamino substituted by substituent(s) independently selected from
    - halogen,
    - nitro,
    - C<sub>1</sub>-C<sub>3</sub> alkyl,
    - C<sub>1</sub>-C<sub>3</sub> alkoxy,
    - halogenated C<sub>1</sub>-C<sub>3</sub> alkoxy,
    - C<sub>1</sub>-C<sub>3</sub> alkoxy,
    - C<sub>1</sub>-C<sub>3</sub> alkoxy substituted by substituent(s) independently selected from
      - halogen,
      - carbocyclic aryl,
      - carbocyclic aryloxy,
      - C<sub>1</sub>-C<sub>3</sub> alkoxy carbonyl,
      - mono- or di-C<sub>1</sub>-C<sub>3</sub> alkylamino,
      - C<sub>1</sub>-C<sub>3</sub> alkylthio,
      - halogenated C<sub>1</sub>-C<sub>3</sub> alkylthio,
      - C<sub>1</sub>-C<sub>3</sub> alkylsulfonyl,
      - C<sub>3</sub>-C<sub>6</sub> cycloalkyl,
      - carbocyclic aryl,
      - heterocyclyl,
      - heterocyclyl,
      - heterocyclyl substituted by substituent(s) independently selected from
        - C<sub>1</sub>-C<sub>3</sub> alkyl,
        - C<sub>1</sub>-C<sub>3</sub> alkoxy,

- C<sub>1</sub>-C<sub>3</sub> alkoxy substituted by carbocyclic aryl,
- carbocyclic aryl,
- halogenated carbocyclic aryl,
- (ii) C<sub>2</sub>-C<sub>8</sub> alkenyl,  
C<sub>2</sub>-C<sub>8</sub> alkenyl substituted by substituent(s) independently selected from
  - halogen,
  - C<sub>1</sub>-C<sub>3</sub> alkoxy,
  - C<sub>1</sub>-C<sub>3</sub> alkoxy substituted by carbocyclic aryl,
  - carbocyclic aryl,
  - carbocyclic aryl substituted by substituent(s) independently selected from
    - halogen,
    - hydroxy,
    - C<sub>1</sub>-C<sub>3</sub> alkoxy,
    - halogenated C<sub>1</sub>-C<sub>3</sub> alkoxy,
    - heterocyclyl,
    - heterocyclyl substituted by nitro,
- (iii) C<sub>2</sub>-C<sub>4</sub> alkynyl,  
C<sub>2</sub>-C<sub>4</sub> alkynyl substituted by carbocyclic aryl,
- (iv) C<sub>3</sub>-C<sub>6</sub> cycloalkyl,  
C<sub>3</sub>-C<sub>6</sub> cycloalkyl substituted by substituent(s) independently selected from
  - C<sub>1</sub>-C<sub>3</sub> alkyl,
  - C<sub>1</sub>-C<sub>3</sub> alkyl substituted by substituent(s) independently selected from
    - hydroxy,
    - oxo,
    - carbocyclic aryl,
    - mono- or di-C<sub>1</sub>-C<sub>3</sub> alkylamino,
    - mono- or di-C<sub>1</sub>-C<sub>3</sub> alkylamino substituted by carbocyclic aryl,
    - carbocyclic aryl,
- (v) C<sub>3</sub>-C<sub>6</sub> cycloalkenyl,  
C<sub>3</sub>-C<sub>6</sub> cycloalkenyl substituted by C<sub>1</sub>-C<sub>3</sub> alkyl,
- (vi) carbocyclyl,  
carbocyclyl substituted by substituent(s) independently selected from

- hydroxy,
- nitro,
- (vii) carbocyclic aryl,
- carbocyclic aryl substituted by substituent(s) independently selected from
  - halogen,
  - hydroxy,
  - cyano,
  - nitro,
  - C<sub>1</sub>-C<sub>9</sub> alkyl,
  - C<sub>1</sub>-C<sub>9</sub> alkyl substituted by substituent(s) independently selected from
    - halogen,
    - hydroxy,
    - oxo,
    - C<sub>1</sub>-C<sub>3</sub> alkoxy,
    - carbocyclic aryloxy,
    - mono- or di-C<sub>1</sub>-C<sub>3</sub> alkylamino-N-oxy,
    - mono- or di-C<sub>1</sub>-C<sub>3</sub> alkylamino,
    - mono- or di-C<sub>1</sub>-C<sub>3</sub> alkylamino substituted by carbocyclic aryl,
    - mono- or di-carbocyclic arylamino,
    - mono- or di-carbocyclic arylamino substituted by C<sub>1</sub>-C<sub>3</sub> alkoxy,
    - carbocyclic aryl,
    - halogenated carbocyclic aryl,
    - heterocyclyl,
    - heterocyclyl substituted by C<sub>1</sub>-C<sub>3</sub> alkyl,
    - C<sub>2</sub>-C<sub>3</sub> alkenyl,
    - C<sub>2</sub>-C<sub>3</sub> alkenyl substituted by carbocyclic aryl,
    - C<sub>1</sub>-C<sub>9</sub> alkoxy,
    - C<sub>1</sub>-C<sub>9</sub> alkoxy substituted by substituent(s) independently selected from
      - hydroxy,
      - halogen,
      - carboxy,
      - mono- or di-C<sub>1</sub>-C<sub>3</sub> alkylamino,

- carbocyclic aryl,
- halogenated carbocyclic aryl,
- heterocyclyl,
- heterocyclyl substituted by substituent(s) independently selected from
- heterocyclyl,
- heterocyclyl substituted by substituent(s) independently selected from
- halogen,
- C<sub>1</sub>-C<sub>3</sub> alkyl,
- halogenated C<sub>1</sub>-C<sub>3</sub> alkyl,
- C<sub>2</sub>-C<sub>3</sub> alkenyloxy,
- C<sub>1</sub>-C<sub>3</sub> alkylcarbonyloxy,
- carbocyclic aryloxy,
- carbocyclic aryloxy substituted by substituent(s) independently selected from
- halogen,
- C<sub>1</sub>-C<sub>4</sub> alkyl,
- halogenated C<sub>1</sub>-C<sub>4</sub> alkyl,
- C<sub>1</sub>-C<sub>3</sub> alkoxy,
- heterocyclyloxy,
- heterocyclyloxy substituted by substituent(s) independently selected from
- halogen,
- C<sub>1</sub>-C<sub>3</sub> alkyl,
- halogenated C<sub>1</sub>-C<sub>3</sub> alkyl,
- (carbocyclic aryl)S(O)<sub>2</sub>O,
- carboxy,
- C<sub>1</sub>-C<sub>3</sub> alkoxycarbonyl,
- mono- or di-C<sub>1</sub>-C<sub>3</sub> alkylaminocarbonyl,
- mono- or di-C<sub>1</sub>-C<sub>3</sub> alkylaminocarbonyl substituted by carbocyclic aryl,
- amino,
- mono- or di-C<sub>1</sub>-C<sub>4</sub> alkylamino,
- mono- or di-C<sub>1</sub>-C<sub>4</sub> alkylamino substituted by cyano,
- mono- or di-carbocyclic arylamino,
- C<sub>1</sub>-C<sub>3</sub> alkylcarbonylamino,

- carbocyclic arylsulfonylamino,
- carbocyclic arylsulfonylamino substituted by C<sub>1</sub>-C<sub>3</sub> alkyl,
- (carbocyclic aryl)NHC(O)NH,
- (carbocyclic aryl)NHC(O)NH substituted by C<sub>1</sub>-C<sub>3</sub> alkoxy,
- (carbocyclic aryl)NHC(O)NH substituted by halogenated C<sub>1</sub>-C<sub>3</sub> alkoxy,
- C<sub>1</sub>-C<sub>3</sub> alkylthio,
- halogenated C<sub>1</sub>-C<sub>3</sub> alkylthio,
- carbocyclic arylthio,
- halogenated carbocyclic arylthio,
- carbocyclic arylthio substituted by C<sub>1</sub>-C<sub>3</sub> alkyl,
- heterocyclylthio,
- C<sub>1</sub>-C<sub>3</sub> alkylsulfonyl,
- mono- or di-C<sub>1</sub>-C<sub>3</sub> alkylaminosulfonyl,
- carbocyclic aryl,
- carbocyclic aryl substituted by substituent(s) independently selected from
  - C<sub>1</sub>-C<sub>7</sub> alkyl,
  - halogenated C<sub>1</sub>-C<sub>7</sub> alkyl,
  - heterocyclyl,
  - heterocyclyl substituted by substituent(s) independently selected from
    - C<sub>1</sub>-C<sub>3</sub> alkyl,
    - carbocyclic aryl,
    - halogenated carbocyclic aryl,
- (viii) heterocyclyl,  
or heterocyclyl substituted by substituent(s) independently selected from
  - halogen,
  - hydroxy,
  - cyano,
  - nitro,
  - C<sub>1</sub>-C<sub>4</sub> alkyl,
  - C<sub>1</sub>-C<sub>4</sub> alkyl substituted by substituent(s) independently selected from
    - halogen,
    - hydroxy,

- oxo,
- C<sub>1</sub>-C<sub>3</sub> alkylcarbonyloxy,
- C<sub>1</sub>-C<sub>3</sub> alkoxycarbonyl,
- C<sub>1</sub>-C<sub>3</sub> alkylthio,
- C<sub>1</sub>-C<sub>3</sub> alkylthio substituted by carbocyclic aryl,
- C<sub>1</sub>-C<sub>3</sub> alkylthio substituted by halogenated carbocyclic aryl,
- carbocyclic aryl,
- carbocyclic aryl substituted by substituent(s) independently selected from
  - halogen,
  - nitro,
  - heterocyclyl,
  - C<sub>1</sub>-C<sub>3</sub> alkoxy,
  - C<sub>1</sub>-C<sub>3</sub> alkoxy substituted by carbocyclic aryl,
  - carbocyclic aryloxy,
  - carbocyclic aryloxy substituted by C<sub>1</sub>-C<sub>3</sub> alkyl,
  - mono- or di-C<sub>1</sub>-C<sub>3</sub> alkylamino,
  - C<sub>1</sub>-C<sub>4</sub> alkylcarbonylamino,
  - C<sub>1</sub>-C<sub>3</sub> alkylthio,
  - carbocyclic arylthio,
  - halogenated carbocyclic arylthio,
  - carbocyclic arylthio substituted by C<sub>1</sub>-C<sub>3</sub> alkoxycarbonyl,
  - heterocyclylthio,
  - heterocyclylthio substituted by C<sub>1</sub>-C<sub>3</sub> alkyl,
  - C<sub>1</sub>-C<sub>3</sub> alkylsulfonyl,
  - carbocyclic arylsulfonyl,
  - carbocyclic arylsulfonyl substituted by C<sub>1</sub>-C<sub>4</sub> alkyl,
  - C<sub>1</sub>-C<sub>3</sub> alkoxycarbonyl,
  - carbocyclic aryl,
  - carbocyclic aryl substituted by substituent(s) independently selected from
    - halogen,
    - nitro,
    - C<sub>1</sub>-C<sub>3</sub> alkyl,



- halogenated C<sub>1</sub>-C<sub>3</sub> alkyl,
- C<sub>1</sub>-C<sub>3</sub> alkoxy,
- halogenated C<sub>1</sub>-C<sub>3</sub> alkoxy,
- heterocyclyl,
- heterocyclyl substituted by substituent(s) independently selected from
- C<sub>1</sub>-C<sub>3</sub> alkyl,
- halogenated C<sub>1</sub>-C<sub>3</sub> alkyl,
- C<sub>1</sub>-C<sub>3</sub> alkoxy,
- C<sub>1</sub>-C<sub>3</sub> alkoxycarbonyl;

Y is  $-(CH_2)_m$ , m is 0 or 1;

wherein carbocyclic aryl is phenyl, naphthyl, biphenyl, or phenanthryl;

carbocyclyl is 9H-fluorenyl, 9-oxo-fluorenyl, acenaphthyl, anthraquinonyl, indanyl, or indenyl;

heterocyclyl is 1,2,3-thiadiazolyl, 1,2,3-triazolyl, 1,2-dihydro-3-oxo-pyrazolyl, 1,3,4-thiadiazolyl, 1,3-dioxo-isoindolyl, 1,3-dioxolanyl, 1H-indolyl, 1H-pyrrolo[2,3-c]pyridyl, 1H-pyrrolyl, 2,2',5',2"-terthiophenyl, 2,2'-bithiophenyl, 2,3-dihydro-1-oxo-isoindolyl, 2,3-dihydro-benzo[1,4]dioxinyl, 2,3-dihydro-benzofuryl, 2,4-dihydro-3-oxo-pyrazolyl, 2H-benzopyranyl, 2-oxo-pyrrolidinyl, 3,4-dihydro-2H-benzo[1,4]oxazinyl, 3,4-dihydro-2H-benzo[b][1,4]dioxepinyl, 4H-benzo[1,3]dioxinyl, 4H-benzopyranyl, 4-oxo-1,5,6,7-tetrahydro-indolyl, 4-oxo-benzopyranyl, 9H-carbazolyl, 9H-xanthenyl, azetidiny, benzimidazolyl, benzo[1,3]dioxolyl, benzo[b]thienyl, benzofuryl, benzothiazolyl, furyl, imidazo[2,1-b]thiazolyl, imidazolyl, isoxazolyl, morpholino, morpholinyl, oxolanyl, piperazyl, piperidyl, pyrazolo[5,1-b]thiazolyl, pyrazolyl, pyridyl, pyrimidyl, pyrrolidyl, quinolyl, quinoxalyl, thiazolidyl, thiazolyl, thienyl, or thiolanyl;

halogen is fluoro, chloro, bromo, or iodo;

or a salt thereof.

11. A compound according to claim 10, wherein

R<sub>1</sub> represents

- (i) C<sub>1</sub>-C<sub>10</sub> alkyl substituted by substituent(s) independently selected from
- methoxy,
- methoxy substituted by carbocyclic aryl,

- carbocyclic aryloxy,
- halogenated carbocyclic aryloxy,
- mono-C<sub>1</sub>-C<sub>2</sub> alkylamino substituted by cyano,
- mono- or di-C<sub>1</sub>-C<sub>2</sub> alkylamino substituted by carbocyclic aryl,
- mono-carbocyclic arylamino,
- mono-carbocyclic arylamino substituted by methyl,
- carbocyclic arylsulfonylamino substituted by methyl,
- carbocyclic aryl,
- carbocyclic aryl substituted by substituent(s) independently selected from
  - halogen,
  - nitro,
  - C<sub>1</sub>-C<sub>4</sub> alkyl,
  - C<sub>1</sub>-C<sub>4</sub> alkyl substituted by carbocyclic aryl,
  - C<sub>1</sub>-C<sub>4</sub> alkyl substituted by hydroxy,
  - C<sub>1</sub>-C<sub>2</sub> alkoxy,
  - halogenated C<sub>1</sub>-C<sub>2</sub> alkoxy,
  - heterocyclyl substituted by carbocyclic aryl,
- (ii) C<sub>2</sub>-C<sub>8</sub> alkenyl substituted by substituent(s) independently selected from
  - methoxy substituted by carbocyclic aryl,
  - carbocyclic aryl,
  - carbocyclic aryl substituted by methoxy,
- (iii) C<sub>2</sub>-C<sub>4</sub> alkynyl substituted by carbocyclic aryl,
- (iv) cyclohexyl substituted by carbocyclic arylmethyl,
- (v) carbocyclyl,
- (vi) carbocyclic aryl,
- carbocyclic aryl substituted by substituent(s) independently selected from
  - halogen,
  - hydroxy,
  - cyano,
  - amino,
  - C<sub>1</sub>-C<sub>9</sub> alkyl,
  - halogenated C<sub>1</sub>-C<sub>9</sub> alkyl,

- C<sub>1</sub>-C<sub>9</sub> alkoxy,
- C<sub>1</sub>-C<sub>9</sub> alkoxy substituted by substituent(s) independently selected from
- halogen,
- halogenated carbocyclic aryl,
- propenyloxy,
- methylamino,
- di-C<sub>1</sub>-C<sub>2</sub> alkylamino,
- di-C<sub>1</sub>-C<sub>2</sub> alkylamino substituted by cyano,
- methylthio,
- halogenated methylthio,
- (vii) heterocyclyl,
- or heterocyclyl substituted by substituent(s) independently selected from
- halogen,
- C<sub>1</sub>-C<sub>4</sub> alkyl,
- C<sub>1</sub>-C<sub>4</sub> alkyl substituted by hydroxy,
- C<sub>1</sub>-C<sub>4</sub> alkyl substituted by carbocyclic aryl,
- methoxy,
- C<sub>1</sub>-C<sub>2</sub> alkoxy carbonyl,
- carbocyclic arylthio substituted by methoxycarbonyl,
- carbocyclic aryl,
- carbocyclic aryl substituted by substituent(s) independently selected from
- halogen,
- halogenated methyl,
- heterocyclyl;

R<sub>2</sub> is methylamino or dimethylamino;

L is selected from Formula Va, VIIIa, or IXa;

wherein carbocyclic aryl is phenyl, naphthyl, biphenyl, or phenanthryl;

carbocyclyl is 9H-fluorenyl, acenaphthyl, or anthraquinonyl;

heterocyclyl is 1,2,3-thiadiazolyl, 1,2,3-triazolyl, 1,2-dihydro-3-oxo-pyrazolyl, 1,3-dioxolanyl, 1H-indolyl, 1H-pyrrolyl, 2,2',5',2"-terthiophenyl, 2,2'-bithiophenyl, 2,3-dihydro-benzo[1,4]dioxinyl, 3,4-dihydro-2H-benzo[1,4]oxazinyl, 4-oxo-benzopyranyl, 9H-carbazolyl, 9H-xanthenyl, benzimidazolyl, benzo[1,3]dioxolyl, benzo[b]thienyl, benzofuryl,

benzothiazolyl, furyl, imidazolyl, isoxazolyl, oxolanyl, pyrazolo[5,1-b]thiazolyl, pyrazolyl, pyridyl, pyrimidyl, quinolyl, quinoxalyl, thiazolidyl, thiazolyl, thienyl, 2*H*-benzopyranyl, 4*H*-benzo[1,3]dioxinyl, azetidiny, imidazo[2,1-b]thiazolyl, morpholinyl, or 2,3-dihydro-benzofuryl;

halogen is fluoro, chloro, bromo, or iodo;  
or a salt thereof.

12. A compound according to claim 11, wherein

R<sub>1</sub> represents

(i) C<sub>1</sub>-C<sub>7</sub> alkyl substituted by substituent(s) independently selected from

- methoxy,
- methoxy substituted by carbocyclic aryl,
- carbocyclic aryloxy,
- halogenated carbocyclic aryloxy,
- mono-ethylamino substituted by cyano,
- di-methylamino substituted by carbocyclic aryl,
- mono-carbocyclic arylamino,
- mono-carbocyclic arylamino substituted by methyl,
- carbocyclic arylsulfonylamino substituted by methyl,
- carbocyclic aryl,
- carbocyclic aryl substituted by substituent(s) independently selected from
  - halogen,
  - nitro,
  - C<sub>1</sub>-C<sub>4</sub> alkyl,
  - C<sub>1</sub>-C<sub>4</sub> alkyl substituted by carbocyclic aryl,
  - C<sub>1</sub>-C<sub>4</sub> alkyl substituted by hydroxy,
  - methoxy,
  - halogenated methoxy,
  - heterocyclyl substituted by carbocyclic aryl,

(ii) C<sub>2</sub>-C<sub>7</sub> alkenyl substituted by substituent(s) independently selected from

- methoxy substituted by carbocyclic aryl,
- carbocyclic aryl,

- carbocyclic aryl substituted by methoxy,
- (iii) butynyl substituted by carbocyclic aryl,
- (iv) cyclohexyl substituted by carbocyclic arylmethyl,
- (v) carbocyclyl,
- (vi) carbocyclic aryl,
- carbocyclic aryl substituted by substituent(s) independently selected from
  - halogen,
  - hydroxy,
  - cyano,
  - amino,
  - C<sub>1</sub>-C<sub>2</sub> alkyl,
  - halogenated methyl,
  - C<sub>1</sub>-C<sub>3</sub> alkoxy,
  - C<sub>1</sub>-C<sub>3</sub> alkoxy substituted by substituent(s) independently selected from
    - halogen,
    - halogenated carbocyclic aryl,
    - propenyloxy,
    - di-C<sub>1</sub>-C<sub>2</sub> alkylamino,
    - di-C<sub>1</sub>-C<sub>2</sub> alkylamino substituted by cyano,
    - methylthio,
    - halogenated methylthio,
- (vii) heterocyclyl,
- or heterocyclyl substituted by substituent(s) independently selected from
  - halogen,
  - C<sub>1</sub>-C<sub>3</sub> alkyl,
  - C<sub>1</sub>-C<sub>3</sub> alkyl substituted by hydroxy,
  - C<sub>1</sub>-C<sub>3</sub> alkyl substituted by carbocyclic aryl,
  - methoxy,
  - ethoxycarbonyl,
  - carbocyclic arylthio substituted by methoxycarbonyl,
  - carbocyclic aryl,
  - carbocyclic aryl substituted by substituent(s) independently selected from

- halogen,
- halogenated methyl,
- heterocyclyl;

L is selected from Formula XX - XXII;

wherein carbocyclic aryl is phenyl, **naphthyl**, or biphenyl;

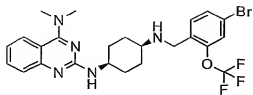
carbocyclyl is acenaphthyl;

heterocyclyl is 1*H*-indolyl, 1*H*-pyrrolyl, 2,3-dihydro-benzo[1,4]dioxinyl, 9*H*-carbazolyl, benzo[1,3]dioxolyl, furyl, pyrazolyl, thienyl, 4-oxo-benzopyranyl, azetidiny, imidazo[2,1-*b*]thiazolyl, pyridyl, imidazolyl, 2,3-dihydro-benzofuryl, or benzo[*b*]thienyl;

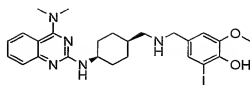
halogen is fluoro, chloro, bromo, or iodo;

or a salt thereof.

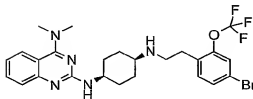
13. A compound according to claim 12 of Formua I selected from the group consisting of



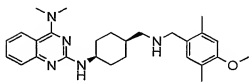
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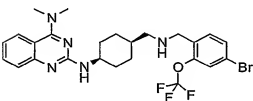
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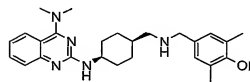
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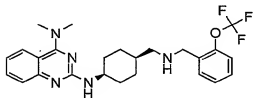
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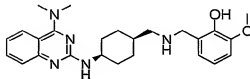
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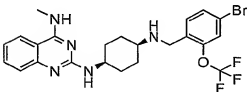
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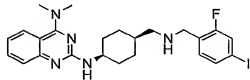
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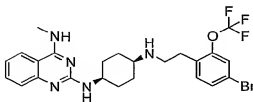
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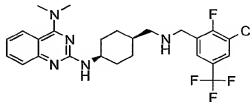
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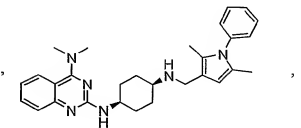
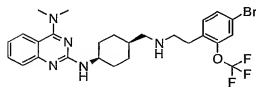
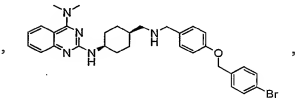
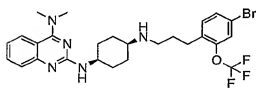
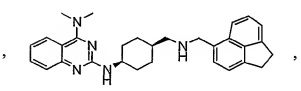
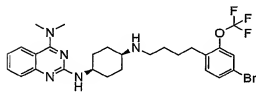
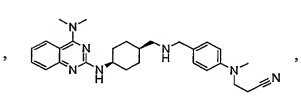
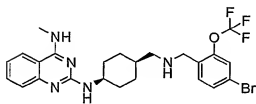
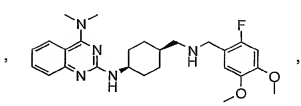
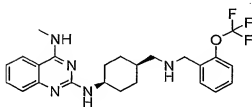
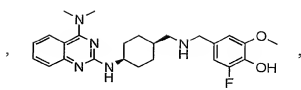
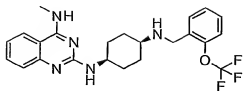
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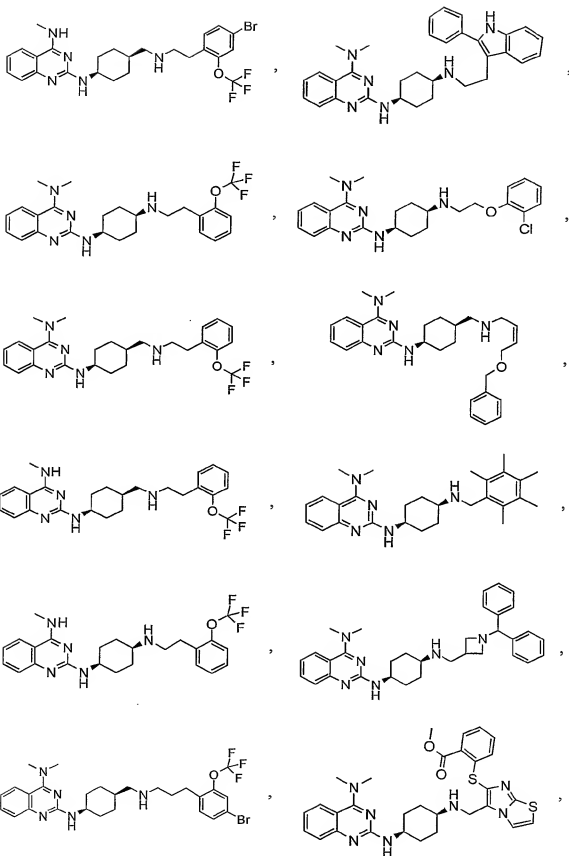
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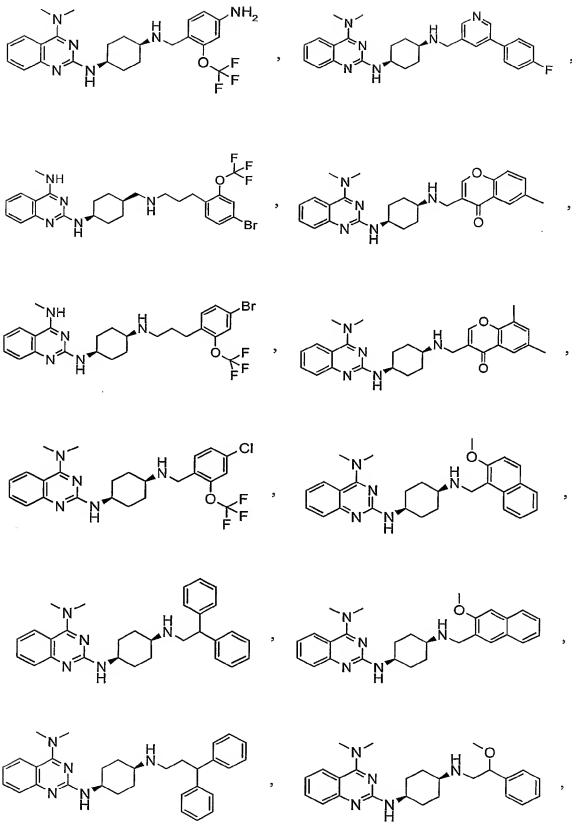


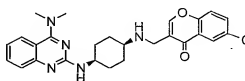
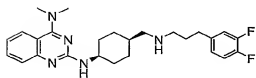
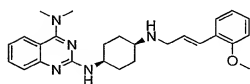
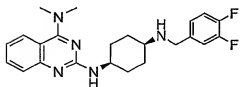
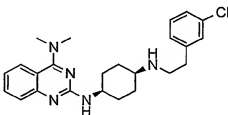
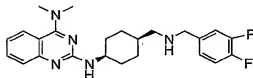
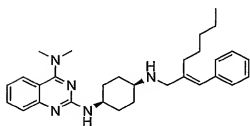
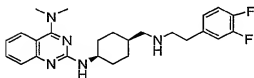
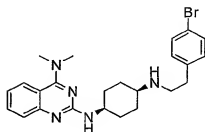
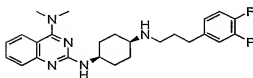
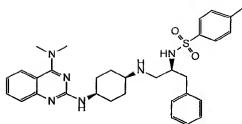
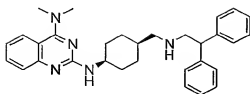
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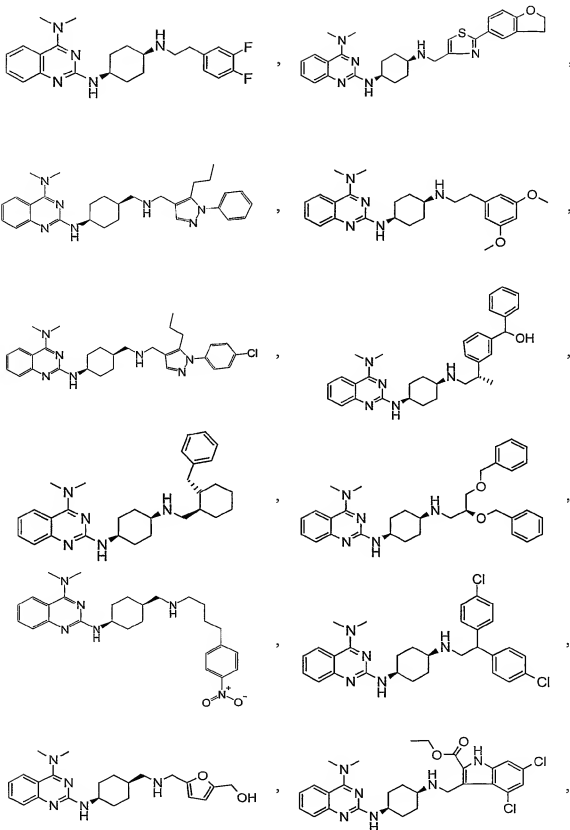


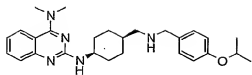




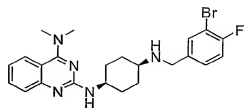




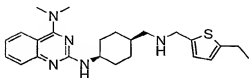




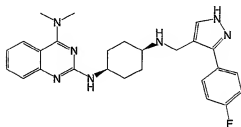
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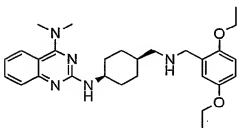
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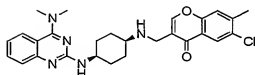
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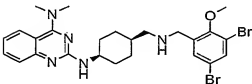
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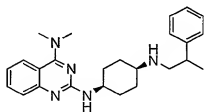
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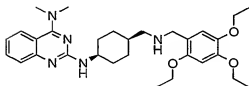
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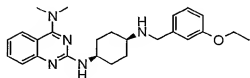
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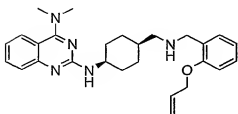
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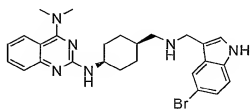
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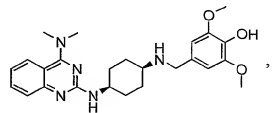
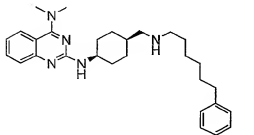
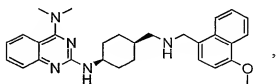
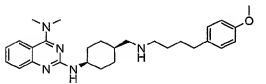
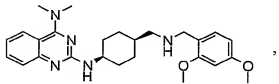
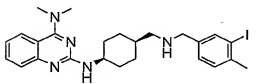
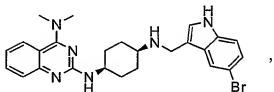
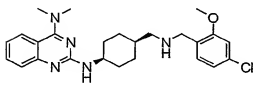
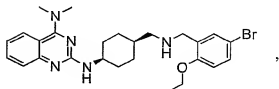
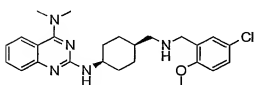
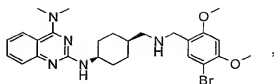
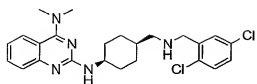


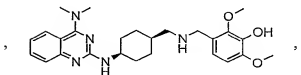
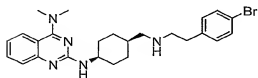
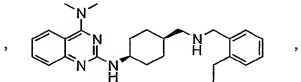
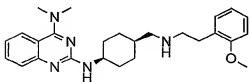
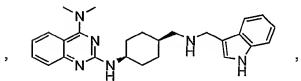
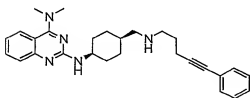
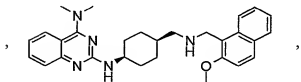
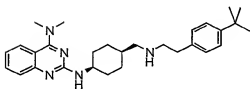
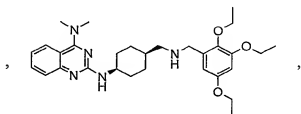
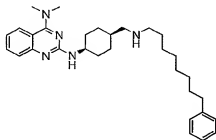
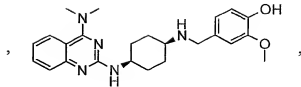
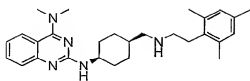
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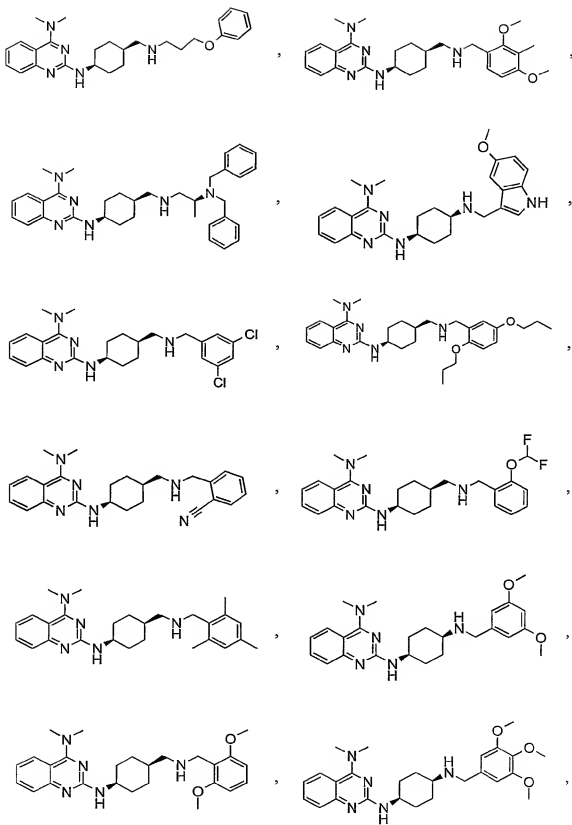
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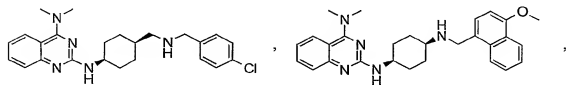
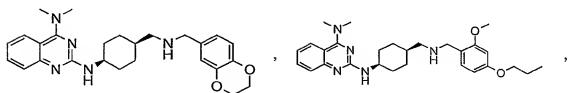
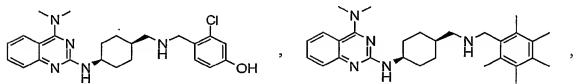
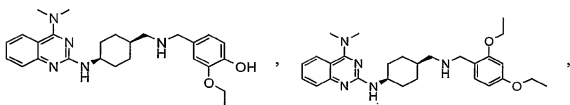
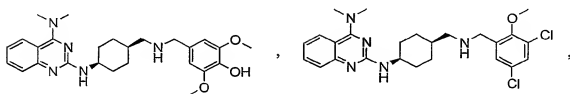
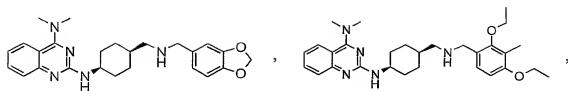


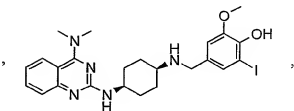
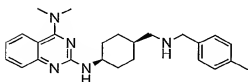
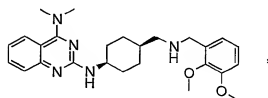
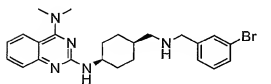
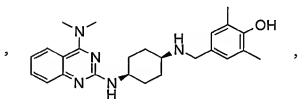
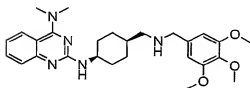
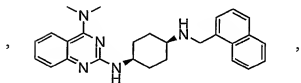
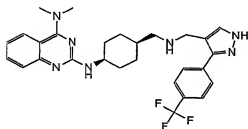
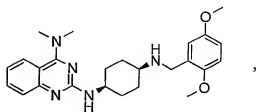
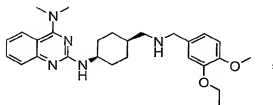
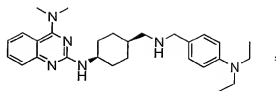
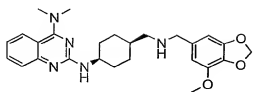


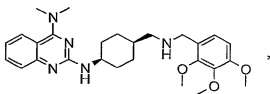
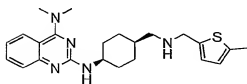
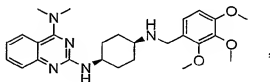
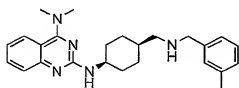
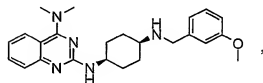
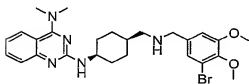
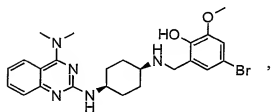
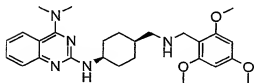
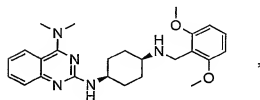
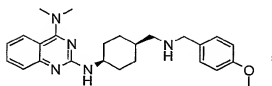
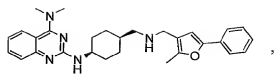
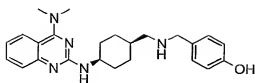


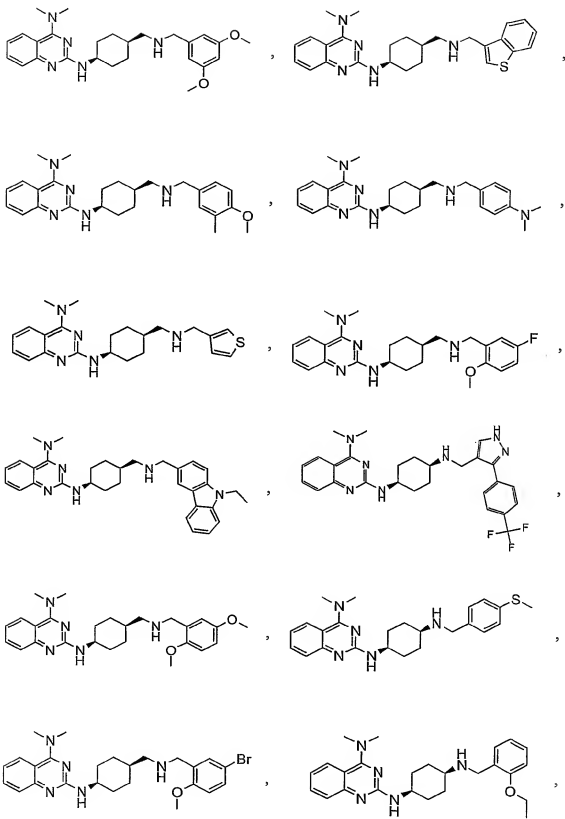


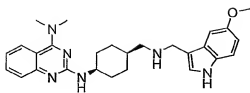




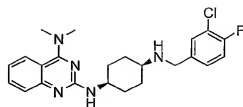




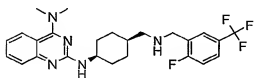




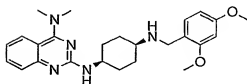
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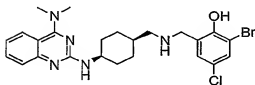
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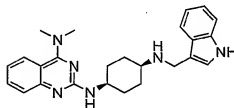
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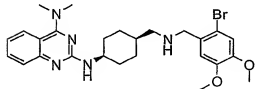
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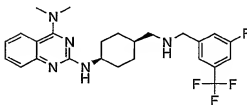
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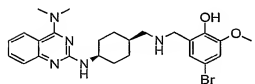
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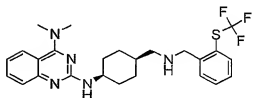
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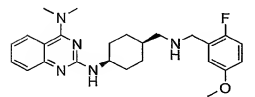
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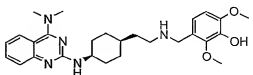
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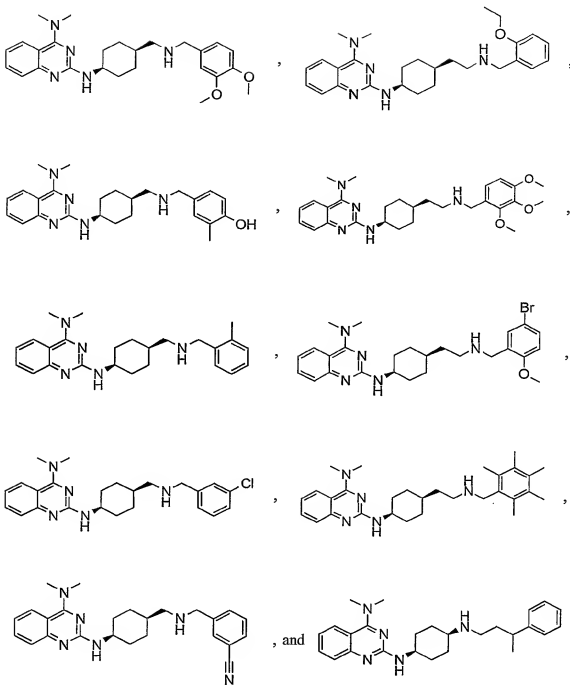
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; or, in case of, a salt thereof.

14. A compound according to claim 1, wherein Q is Formula II;

R<sub>1</sub> represents

(i) C<sub>1</sub>-C<sub>16</sub> alkyl,

C<sub>1</sub>-C<sub>16</sub> alkyl substituted by substituent(s) independently selected from

•halogen,

•carbocyclyl,

•carbocyclic aryl,

•carbocyclic aryl substituted by substituent(s) independently selected from

••halogen,

••nitro,

••C<sub>1</sub>-C<sub>3</sub> alkyl,

••halogenated C<sub>1</sub>-C<sub>3</sub> alkyl,

••C<sub>1</sub>-C<sub>3</sub> alkoxy,

••halogenated C<sub>1</sub>-C<sub>3</sub> alkoxy,

(ii) C<sub>2</sub>-C<sub>3</sub> alkenyl,

C<sub>2</sub>-C<sub>3</sub> alkenyl substituted by carbocyclic aryl,

(iii) carbocyclic aryl,

carbocyclic aryl substituted by substituent(s) independently selected from

•halogen,

•cyano,

•nitro,

•C<sub>1</sub>-C<sub>3</sub> alkyl,

•C<sub>1</sub>-C<sub>3</sub> alkyl substituted by substituent(s) independently selected from

••halogen,

••oxo,

•C<sub>2</sub>-C<sub>3</sub> alkenyl,

•C<sub>1</sub>-C<sub>4</sub> alkoxy,

•C<sub>1</sub>-C<sub>4</sub> alkoxy substituted by substituent(s) independently selected from

••halogen,

••heterocyclyl,

••halogenated heterocyclyl,

•carbocyclic aryloxy,



- carbocyclic aryloxy substituted by substituent(s) independently selected from
  - halogen,
  - nitro,
  - heterocyclyloxy,
- heterocyclyloxy substituted by substituent(s) independently selected from
  - halogen,
  - C<sub>1</sub>-C<sub>3</sub> alkyl,
  - halogenated C<sub>1</sub>-C<sub>3</sub> alkyl,
  - C<sub>1</sub>-C<sub>3</sub> alkoxycarbonyl,
  - mono- or di-C<sub>1</sub>-C<sub>4</sub> alkylamino,
  - C<sub>1</sub>-C<sub>3</sub> alkylcarbonylamino,
  - carbocyclic aryl diazo,
  - carbocyclic aryl diazo substituted by mono- or di- C<sub>1</sub>-C<sub>3</sub> alkylamino,
  - C<sub>1</sub>-C<sub>3</sub> alkylsulfonyl,
  - carbocyclic aryl,
- (iv) heterocyclyl,
  - or heterocyclyl substituted by substituent(s) independently selected from
    - halogen,
    - C<sub>1</sub>-C<sub>3</sub> alkyl,
  - C<sub>1</sub>-C<sub>3</sub> alkyl substituted by substituent(s) independently selected from
    - halogen,
    - oxo,
    - carbocyclic arylcarbonylamino,
    - halogenated carbocyclic arylcarbonylamino,
    - heterocyclyl,
    - heterocyclyl substituted by substituent(s) independently selected from
      - halogen,
      - C<sub>1</sub>-C<sub>3</sub> alkyl,
      - halogenated C<sub>1</sub>-C<sub>3</sub> alkyl,
      - C<sub>1</sub>-C<sub>3</sub> alkoxy,
      - C<sub>1</sub>-C<sub>3</sub> alkylcarbonylamino,
      - carbocyclic arylsulfonyl,

- C<sub>1</sub>-C<sub>3</sub> alkoxycarbonyl,
- carbocyclic aryl,
- halogenated carbocyclic aryl,
- heterocyclyl,
- heterocyclyl substituted by substituent(s) independently selected from
  - halogen,
  - C<sub>1</sub>-C<sub>3</sub> alkyl,
  - halogenated C<sub>1</sub>-C<sub>3</sub> alkyl;

Y is -S(O)<sub>2</sub>-;

wherein carbocyclic aryl is phenyl, biphenyl, or naphthyl;

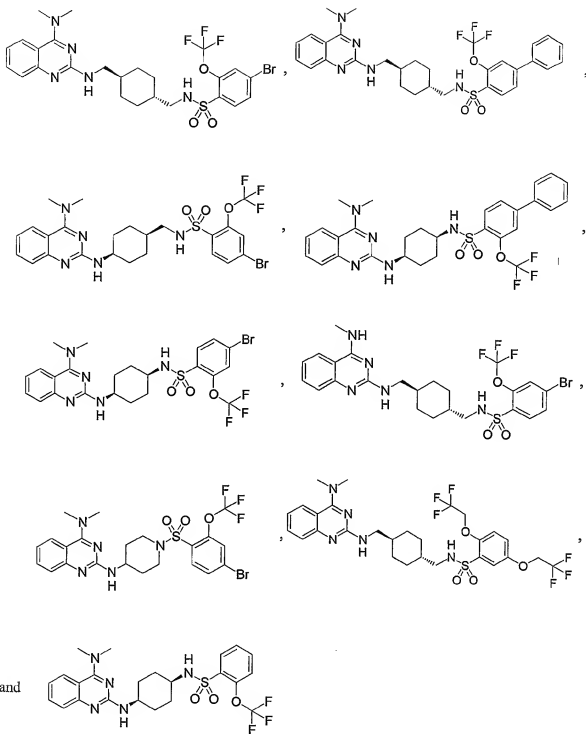
carbocyclyl is 7,7-dimethyl-2-oxo-bicyclo[2.2.1]heptyl;

heterocyclyl is 1,2,3,4-tetrahydro-isoquinolyl, 1,2,3-thiadiazolyl, 1*H*-pyrrolyl, benzo[2,1,3]oxadiazolyl, benzo[b]thienyl, furyl, imidazolyl, isoxazolyl, pyrazolyl, pyridyl, quinolyl, thiazolyl, or thienyl;

halogen is fluoro, chloro, bromo, or iodo;

or a salt thereof.

15. A compound according to claim 14 of Formua I selected from the group consisting of



16. A compound according to claim 1, wherein Q is Formula II;  
R<sub>1</sub> is selected from H, -CO<sub>2</sub>tBu, or -CO<sub>2</sub>Bn (Bn is a benzyl group);  
R<sub>2</sub> is methylamino or dimethylamino;  
L is selected from Formula XX - XXII;  
Y is a single bond;  
or a salt thereof.

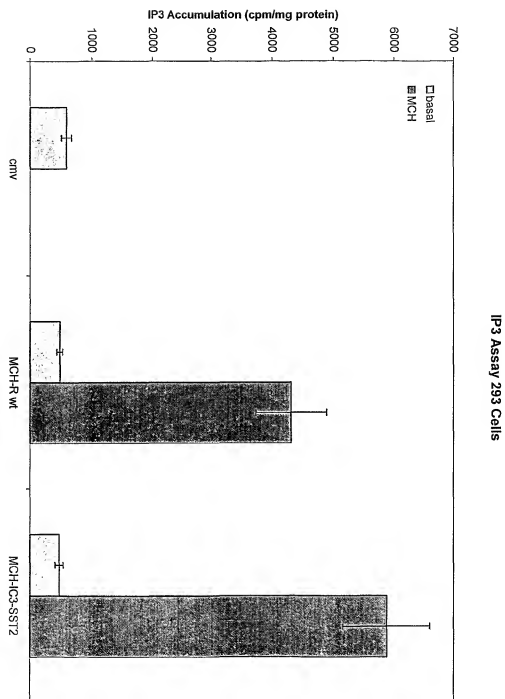
17. A method for modulating the G-protein receptor, SLC-1, comprising the step of contacting said SLC-1 with a MCH receptor antagonist.

18. A method for modulating the G-protein receptor, SLC-1, comprising the step of contacting said SLC-1 with a compound of claims 1-16.

19. The method of prophylaxis or treatment of obesity, obesity related disorders, anxiety, or depression in mammals in need of such treatment comprising administering to the mammal a therapeutically effective amount of a compound having the composition of any of claims 1-16.

20. A pharmaceutical composition comprising a pharmaceutically acceptable carrier and a therapeutically effective amount of a compound having the composition of any of claims 1-16.

Fig. 1



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 Thr Val His Pro Ile Ser Ser Thr Lys Phe Arg Lys Pro Ser Val Ala  
 145 150 155 160  
 Thr Leu Val Ile Cys Leu Leu Trp Ala Leu Ser Phe Ile Ser Ile Thr  
 165 170 175  
 Pro Val Trp Leu Tyr Ala Arg Leu Ile Pro Phe Pro Gly Gly Ala Val  
 180 185 190  
 Gly Cys Gly Ile Arg Leu Pro Asn Pro Asp Thr Asp Leu Tyr Trp Phe  
 195 200 205  
 Thr Leu Tyr Gln Phe Phe Leu Ala Phe Ala Leu Pro Phe Val Val Ile  
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 Thr Ala Ala Tyr Val Arg Ile Leu Gln Lys Val Lys Ser Ser Gly Ile  
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 Arg Val Gly Ser Ser Lys Arg Lys Lys Ser Glu Lys Lys Val Thr Arg  
 245 250 255  
 Thr Ala Ile Ala Ile Cys Leu Val Phe Phe Val Cys Trp Ala Pro Tyr  
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 Tyr Val Leu Gln Leu Thr Gln Leu Ser Ile Ser Arg Pro Thr Leu Thr  
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 Phe Val Tyr Leu Tyr Asn Ala Ala Ile Ser Leu Gly Tyr Ala Asn Ser

290                      295                      300  
 Cys Leu Asn Pro Phe Val Tyr Ile Val Leu Cys Glu Thr Phe Arg Lys  
 305                      310                      315                      320  
 Arg Leu Val Leu Ser Val Lys Pro Ala Ala Gln Gly Gln Leu Arg Ala  
                          325                      330                      335  
 Val Ser Asn Ala Gln Thr Ala Asp Glu Glu Arg Thr Glu Ser Lys Gly  
                          340                      345                      350  
 Thr Tyr Phe Pro Cys His Pro Ala His Leu Gln Val Arg Ala Pro Gln  
                          355                      360                      365  
 His Ala Thr Gly Arg Asp Ala Glu Lys Asn Pro Arg Pro Leu Gly Lys  
                          370                      375                      380  
 Cys Arg Lys Ala Gly Leu Gly Val Val Ala Met Lys Ile His Ser Met  
 385                      390                      395                      400  
 Gly Ser His Val Ala Gly Glu Ala Trp Ser Gln Val Trp Gly Phe Gln  
                          405                      410                      415  
 Ile Ser Glu Ile Pro Trp Gly Ser Arg Met Arg Pro Leu Asp Arg Thr  
                          420                      425                      430  
 Glu Ala Glu Gln Glu Asn Met Leu Val Trp Ile Thr Gly Cys  
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&lt;213&gt; Artificial

&lt;220&gt;

&lt;223&gt; Novel Sequence

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&lt;213&gt; Artificial

&lt;220&gt;

&lt;223&gt; Novel Sequence

&lt;400&gt; 8

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accttctgca g 71

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&lt;211&gt; 30

&lt;212&gt; DNA

&lt;213&gt; Artificial

&lt;220&gt;

&lt;223&gt; Novel Sequence

&lt;400&gt; 9

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&lt;211&gt; 24

&lt;212&gt; DNA

&lt;213&gt; Artificial

&lt;220&gt;

&lt;223&gt; Novel Sequence

&lt;400&gt; 10

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&lt;210&gt; 11

&lt;211&gt; 2133

&lt;212&gt; DNA

&lt;213&gt; Homo Sapien

&lt;400&gt; 11

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<212> PRT
<213> Homo Sapien

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Thr Gly Ser Ile Ser Tyr Ile Asn Ile Ile Met Pro Ser Val Phe Gly
 35           40           45

Thr Ile Cys Leu Leu Gly Ile Ile Gly Asn Ser Thr Val Ile Phe Ala
 50           55           60

Val Val Lys Lys Ser Lys Leu His Trp Cys Asn Asn Val Pro Asp Ile
 65           70           75           80

Phe Ile Ile Asn Leu Ser Val Val Asp Leu Leu Phe Leu Leu Gly Met
 85           90           95

Pro Phe Met Ile His Gln Leu Met Gly Asn Gly Val Trp His Phe Gly
100           105           110

Glu Thr Met Cys Thr Leu Ile Thr Ala Met Asp Ala Asn Ser Gln Phe
115           120           125

Thr Ser Thr Tyr Ile Leu Thr Ala Met Ala Ile Asp Arg Tyr Leu Ala
130           135           140

Thr Val His Pro Ile Ser Ser Thr Lys Phe Arg Lys Pro Ser Val Ala
145           150           155           160

Thr Leu Val Ile Cys Leu Leu Trp Ala Leu Ser Phe Ile Ser Ile Thr
165           170           175

Pro Val Trp Leu Tyr Ala Arg Leu Ile Pro Phe Pro Gly Gly Ala Val
180           185           190

Gly Cys Gly Ile Arg Leu Pro Asn Pro Asp Thr Asp Leu Tyr Trp Phe
195           200           205

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Thr Leu Tyr Gln Phe Phe Leu Ala Phe Ala Leu Pro Phe Val Val Ile  
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 Thr Ala Ala Tyr Val Arg Ile Leu Gln Arg Met Thr Ser Ser Val Ala  
 225 230 235 240  
 Pro Ala Ser Gln Arg Ser Ile Arg Leu Arg Thr Lys Arg Val Thr Arg  
 245 250 255  
 Thr Ala Ile Ala Ile Cys Leu Val Phe Phe Val Cys Trp Ala Pro Tyr  
 260 265 270  
 Tyr Val Leu Gln Leu Thr Gln Leu Ser Ile Ser Arg Pro Thr Leu Thr  
 275 280 285  
 Phe Val Tyr Leu Tyr Asn Ala Ala Ile Ser Leu Gly Tyr Ala Asn Ser  
 290 295 300  
 Cys Leu Asn Pro Phe Val Tyr Ile Val Leu Cys Glu Thr Phe Arg Lys  
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 Arg Leu Val Leu Ser Val Lys Pro Ala Ala Gln Gly Gln Leu Arg Ala  
 325 330 335  
 Val Ser Asn Ala Gln Thr Ala Asp Glu Glu Arg Thr Glu Ser Lys Gly  
 340 345 350  
 Thr Ser Arg Met Gly Cys Thr Leu Ser Ala Glu Asp Lys Ala Ala Val  
 355 360 365  
 Glu Arg Ser Lys Met Ile Asp Arg Asn Leu Arg Glu Asp Gly Glu Lys  
 370 375 380  
 Ala Ala Arg Glu Val Lys Leu Leu Leu Leu Gly Ala Gly Glu Ser Gly  
 385 390 395 400  
 Lys Ser Thr Ile Val Lys Gln Met Lys Ile Ile His Glu Ala Gly Tyr  
 405 410 415  
 Ser Glu Glu Glu Cys Lys Gln Tyr Lys Ala Val Val Tyr Ser Asn Thr  
 420 425 430  
 Ile Gln Ser Ile Ile Ala Ile Ile Arg Ala Met Gly Arg Leu Lys Ile  
 435 440 445  
 Asp Phe Gly Asp Ala Ala Arg Ala Asp Asp Ala Arg Gln Leu Phe Val  
 450 455 460  
 Leu Ala Gly Ala Ala Glu Glu Gly Phe Met Thr Ala Glu Leu Ala Gly  
 465 470 475 480  
 Val Ile Lys Arg Leu Trp Lys Asp Ser Gly Val Gln Ala Cys Phe Asn  
 485 490 495  
 Arg Ser Arg Glu Tyr Gln Leu Asn Asp Ser Ala Ala Tyr Tyr Leu Asn  
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Asp Leu Asp Arg Ile Ala Gln Pro Asn Tyr Ile Pro Thr Gln Gln Asp  
 515 520 525  
 Val Leu Arg Thr Arg Val Lys Thr Thr Gly Ile Val Glu Thr His Phe  
 530 535 540  
 Thr Phe Lys Asp Leu His Phe Lys Met Phe Asp Val Gly Gly Gln Arg  
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 Ser Glu Arg Lys Lys Trp Ile His Cys Phe Glu Gly Val Thr Ala Ile  
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 Ile Phe Cys Val Ala Leu Ser Asp Tyr Asp Leu Val Leu Ala Glu Asp  
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 Glu Glu Met Asn Arg Met His Glu Ser Met Lys Leu Phe Asp Ser Ile  
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 Lys Lys Asp Leu Phe Glu Glu Lys Ile Lys Lys Ser Pro Leu Thr Ile  
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 Cys Tyr Pro Glu Tyr Ala Gly Ser Asn Thr Tyr Glu Glu Ala Ala Ala  
 645 650 655  
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 Glu Ile Tyr Thr His Phe Thr Cys Ala Thr Asp Thr Lys Asn Val Gln  
 675 680 685  
 Phe Val Phe Asp Ala Val Thr Asp Val Ile Ile Lys Asn Asn Leu Lys  
 690 695 700  
 Asp Cys Gly Leu Phe  
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